OpenRBC

Redefining the Frontier of Red Blood Cell Simulations at Protein Resolution

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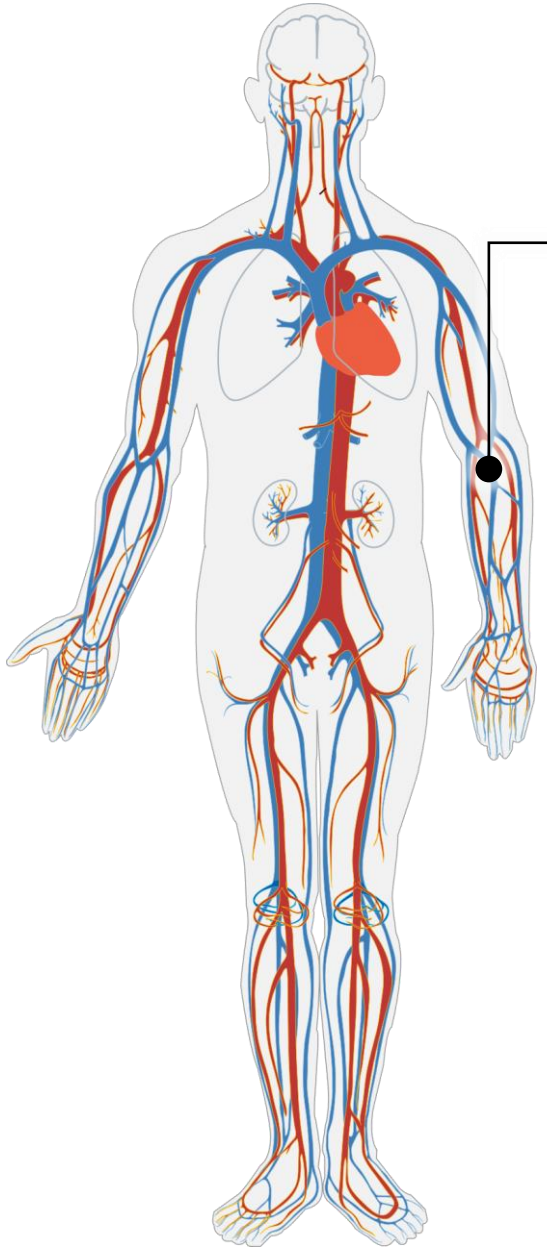
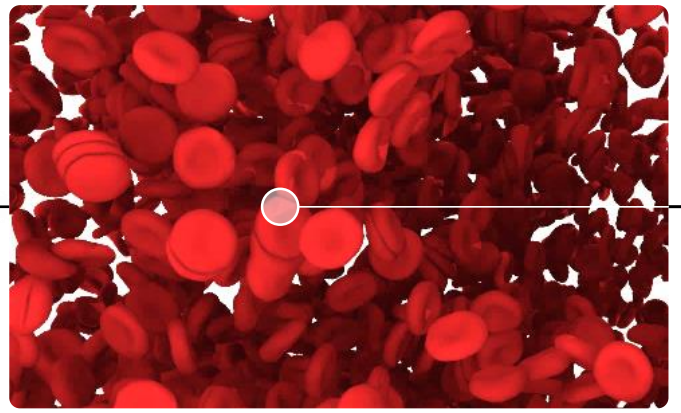
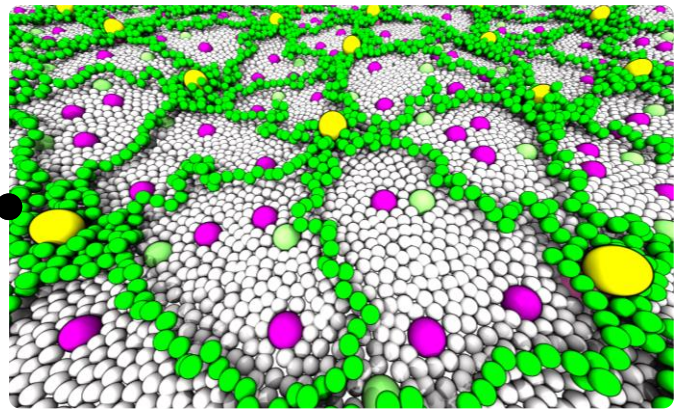
Red Blood Cell (RBC) in Human Body







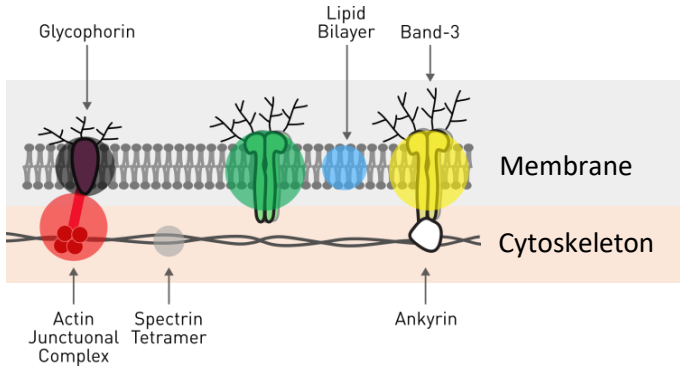
- Most common blood cell
  - 40-45% blood volume (hematocrit)
  - ¼ of total cell count in human body
- Oxygen transport
  - Hemoglobin
- Cell membrane
  - deformability & stability while traveling through the capillary network
- Health: biconcave disks; Diseased: sickle, spherocyte, etc.

Probing RBC Cytomechanics Through Computational Modeling

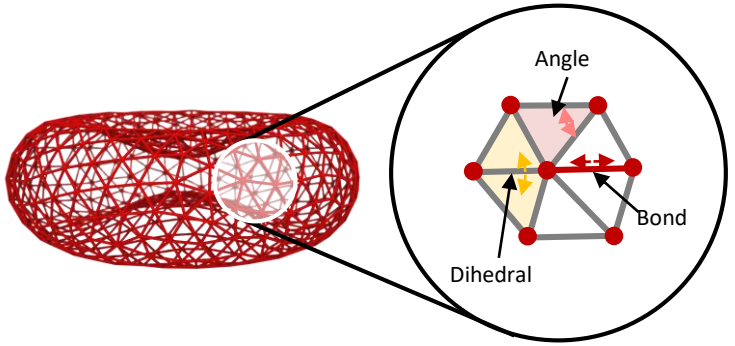
› Quantify properties from structure

› Obtain details of non-Newtonian hydrodynamics

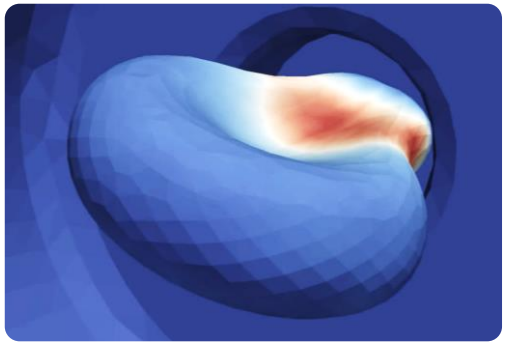
MICROSCOPIC → MESOSCOPIC → CONTINUUM



Li, Biophysical J, 2014



Li, Li, Chang, Lykotrafitis, Karniadakis, 2016



http://fessrg.ucsd.edu/

	MICROSCOPIC	MESOSCOPIC	CONTINUUM
Computational Cost	High	Medium	Low
Level of Detail	High	Medium	Low
Constitutive Equation	Output	Output	Input
Transferability	High	Medium	Low

The OpenRBC Project

› To bridge the gap between microscopic and mesoscopic RBC models

Application	Optical Tweezers	Membrane Fluctuation	Vesiculation	…

› Challenge

To simulate an RBC membrane by

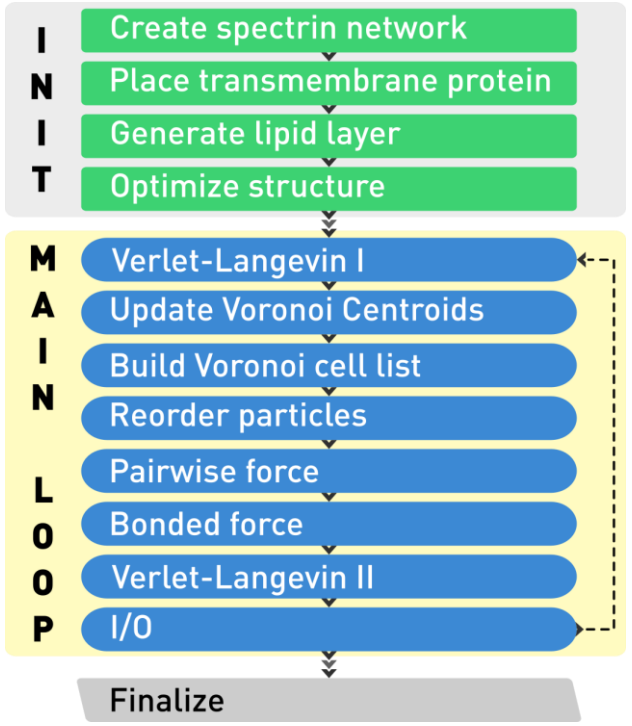
4,000,000
particles

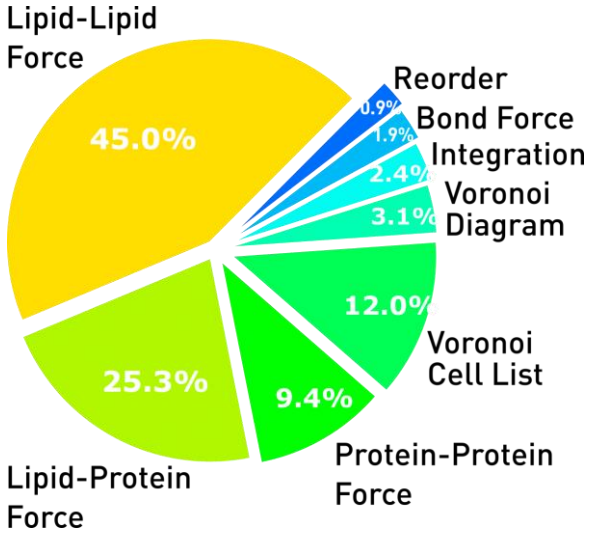
For

1,000,000
time steps

Using

1
node∧day

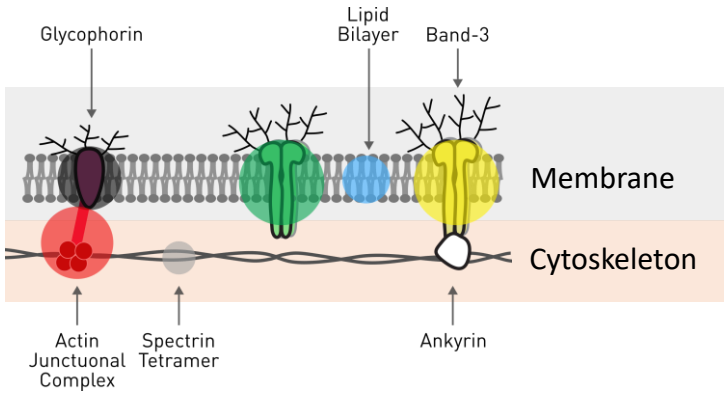


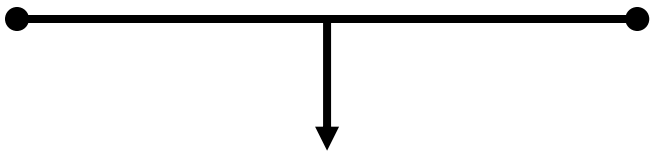


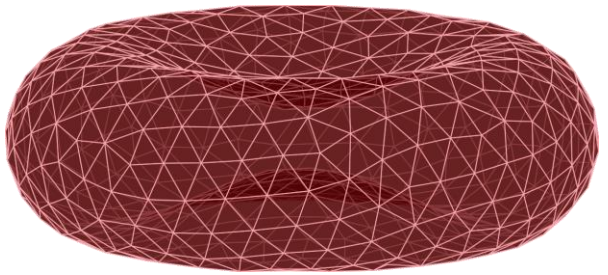
http://openrbc.io/

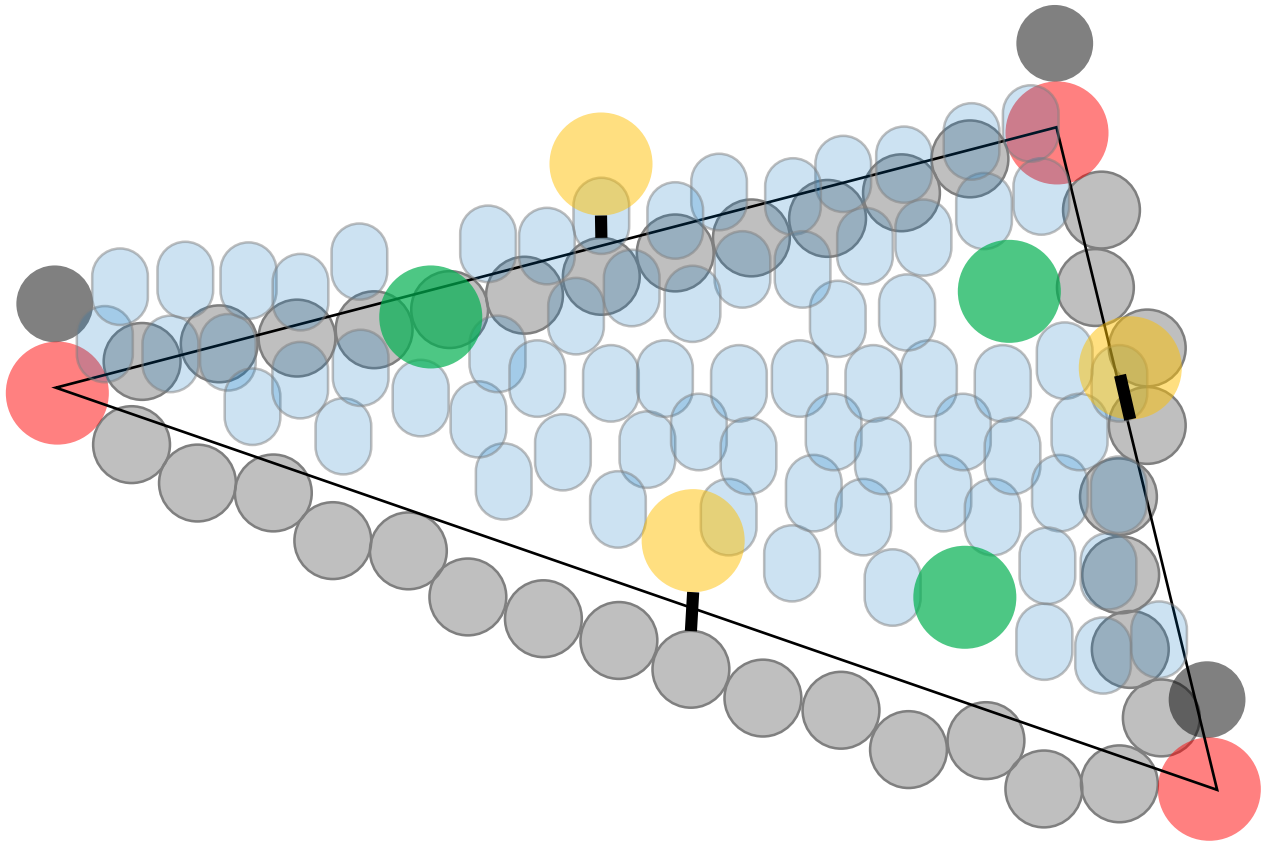
Tang, Lu, Li, Evangelinos, Grinberg, Sachdeva, Karniadakis, *Biophys. J*, 2017.

Model Initialization









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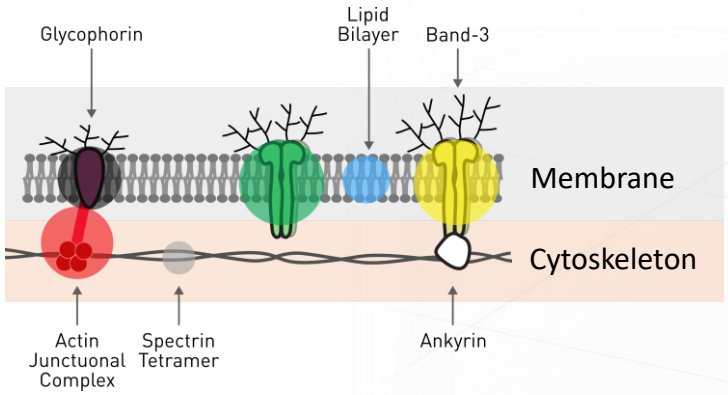
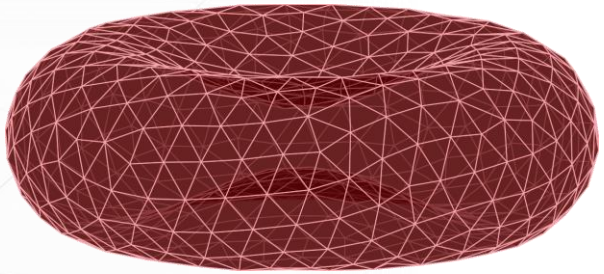
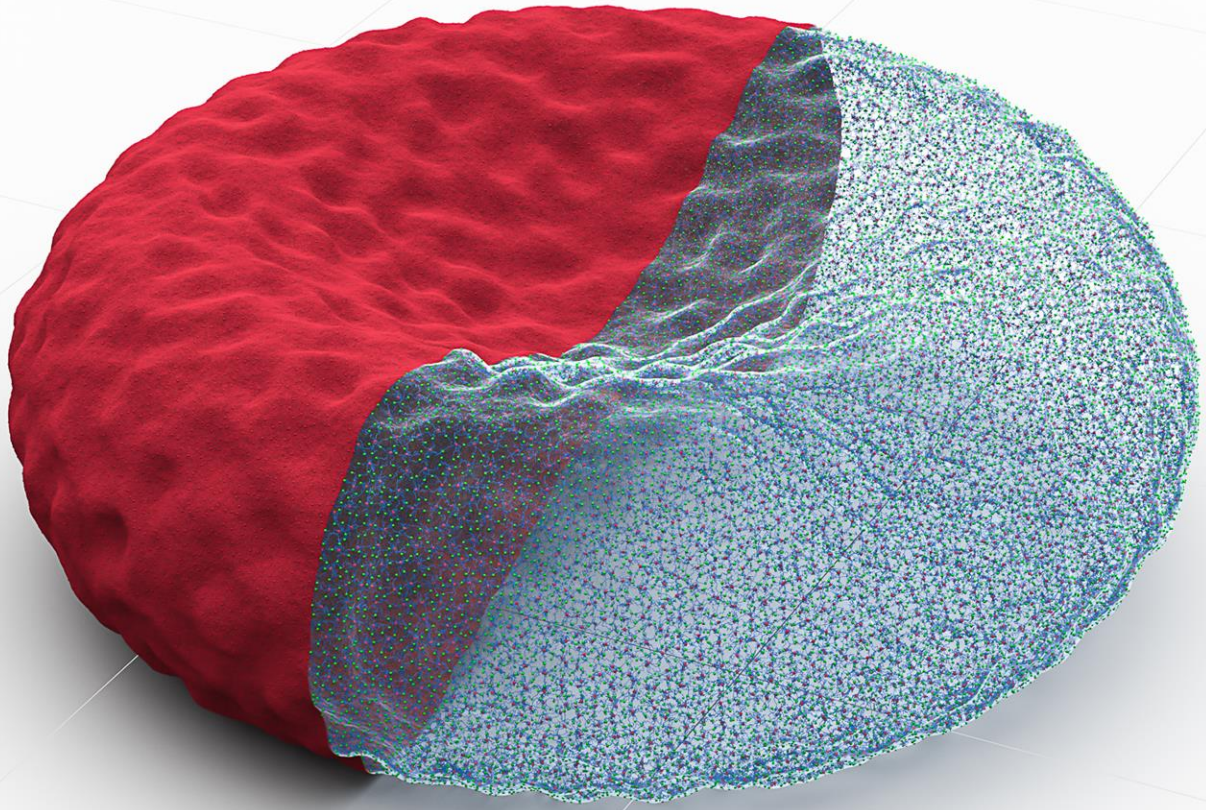
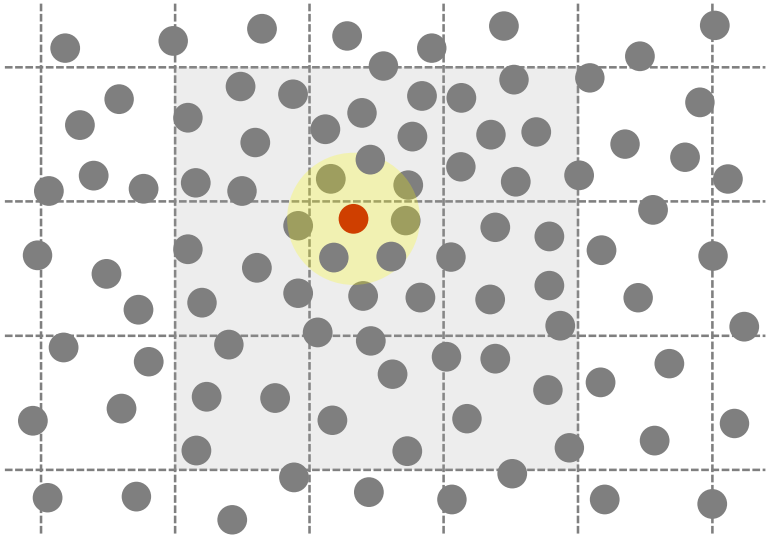


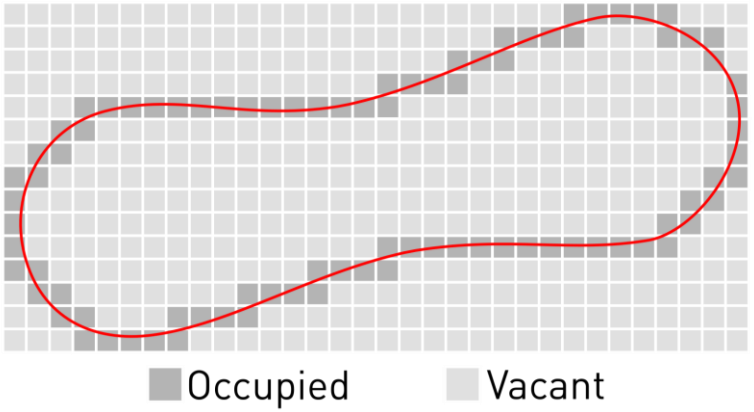




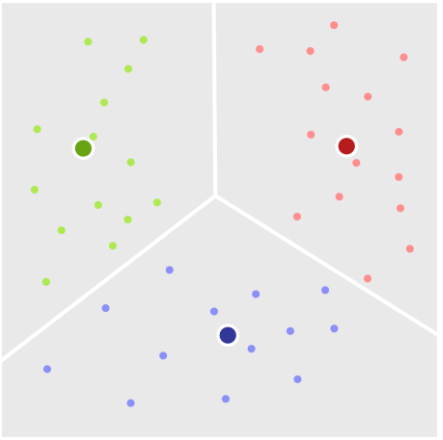
Density Imbalance & Adaptive Partitioning

Cell list



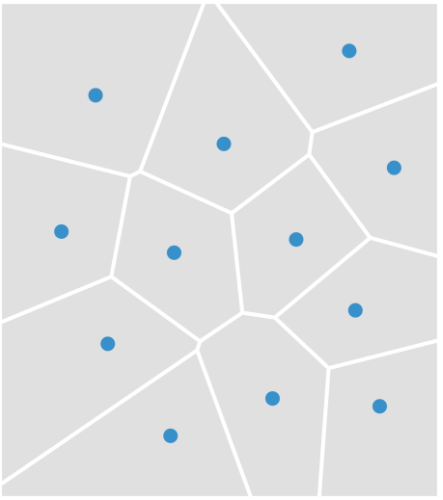


K-means clustering



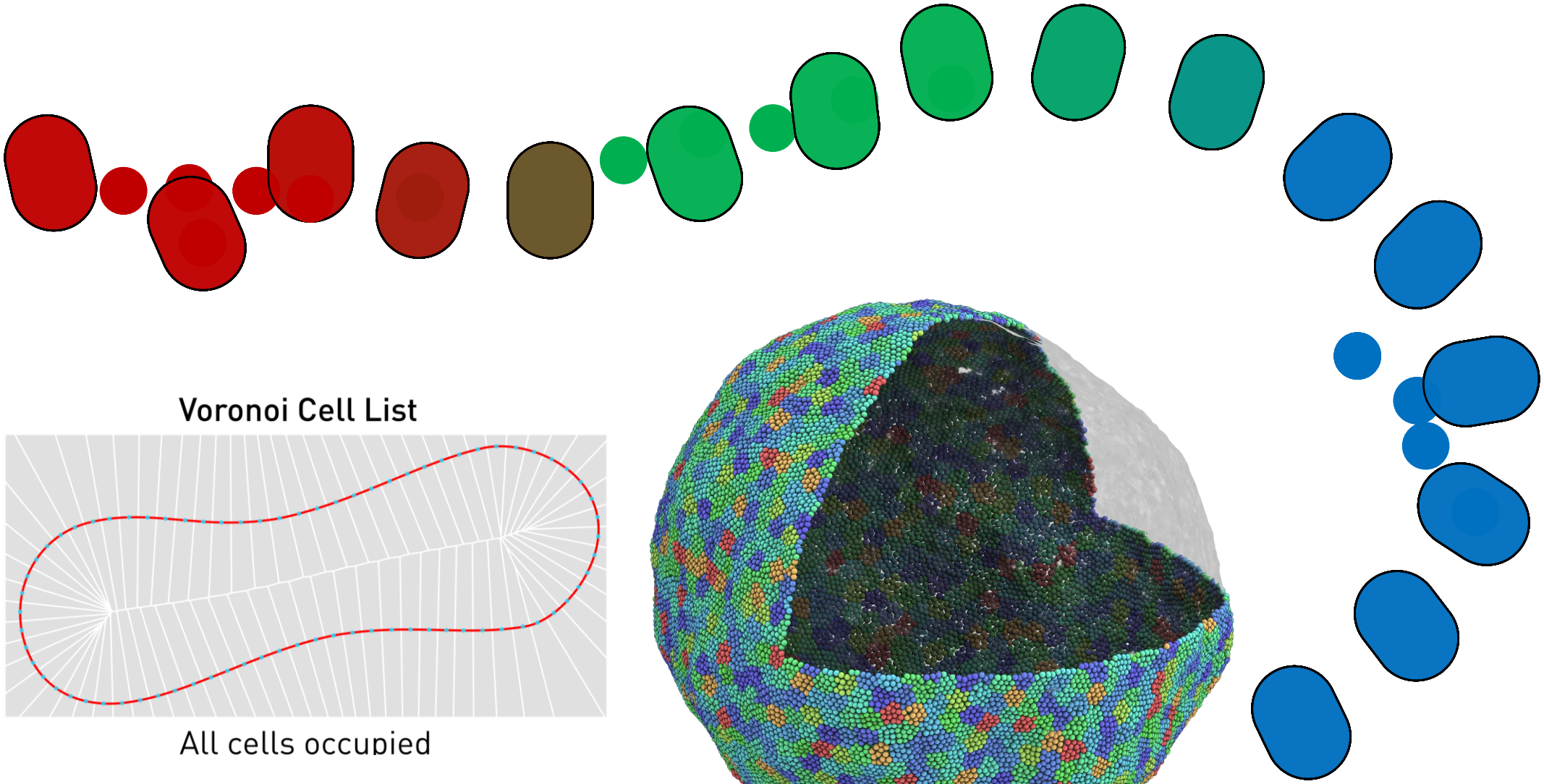
- Divides n vectors into k clusters
- Minimizes within-cluster sum of square distance
- Optimal solution NP-hard
- Iterative heuristics using Expectation-Maximization

Voronoi tessellation



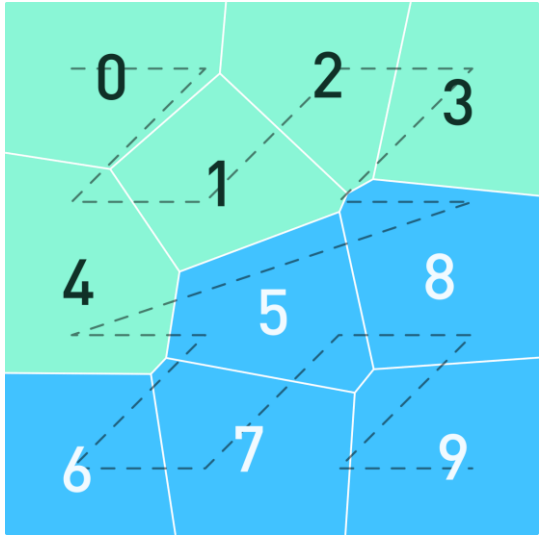
- Each point in the space attributed to the closest centroid
- Continuous version of k-means clustering

Adaptive Partition through k-means Clustering



Parallelization – OpenMP/Vectorization

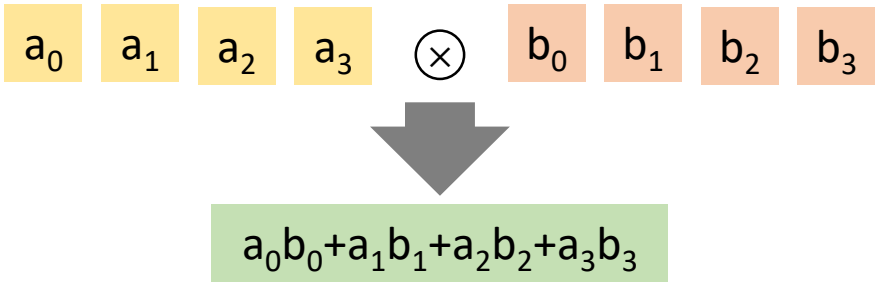
- Divide Voronoi cells into patches
  - Reorder particles by Morton curve to minimize patch boundary contour



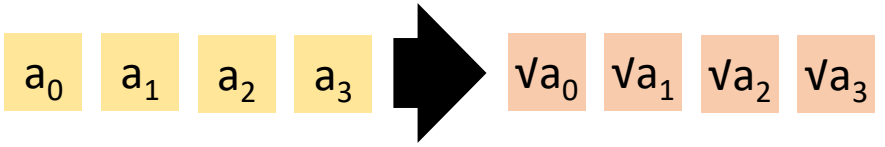
- Force computation
  - intra-patch: once by owner thread
  - inter-patch: twice by each thread

- Explicit vectorization with SSE intrinsics

```
struct vec4f { union { __m128 m128; float x[4]; }; };
```



DPPS: dot product



SQRTPS: square root

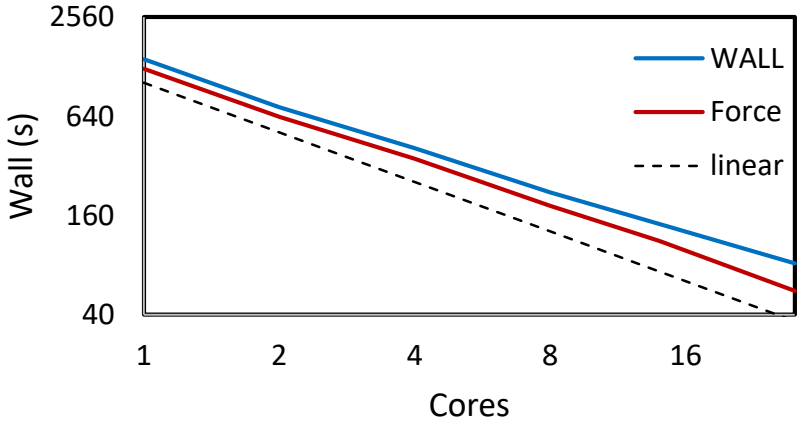
- Implicit vectorization with Altivec
  - Accumulate force computation into vectorizable loops

Benchmark

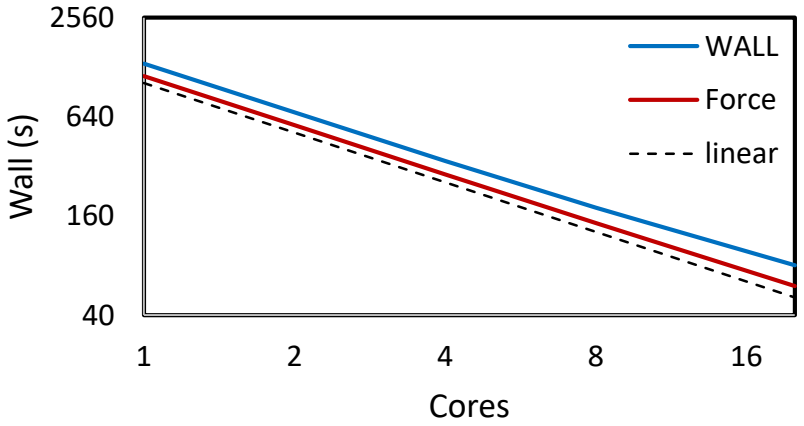
CPU	ISA	Cores	SMT	Total Threads	LLC	GFLOPS	Achieved Peak	Memory BW
Minsky	Power	20	8	160	80×2	560	8.7%	230 GB/s
OLCF Rhea	x86	28	2	56	35×2	1030	4.6%	136 GB/s

Scalability - Core

10^3 steps, Xeon 28-core

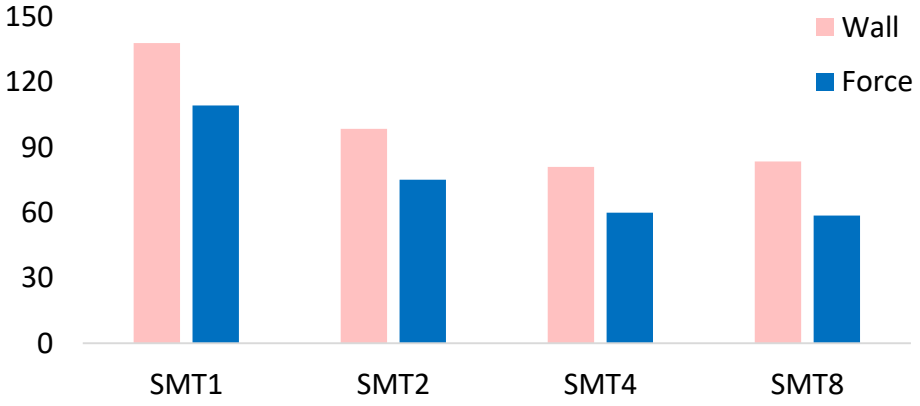


10^3 steps, Power8 20-core

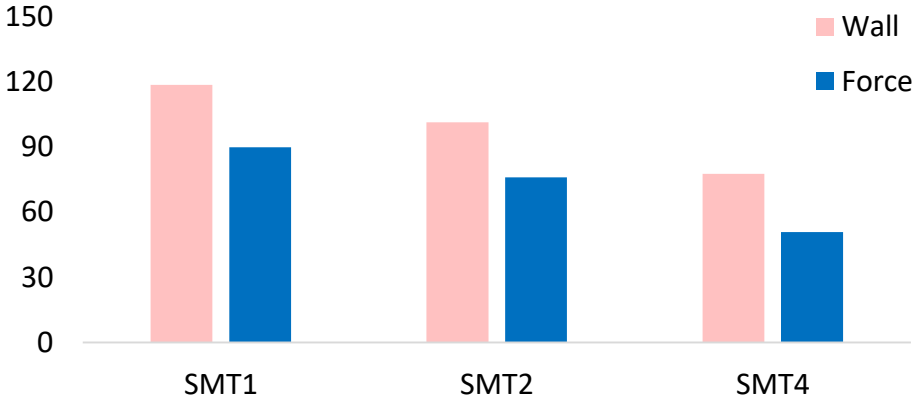


Scalability - SMT

10^3 steps, Power8 20-core

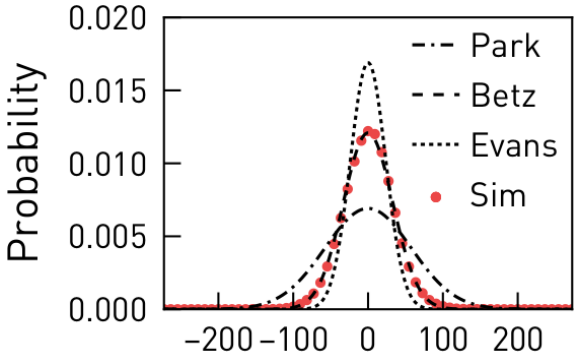


10^3 steps, Power7 32-core



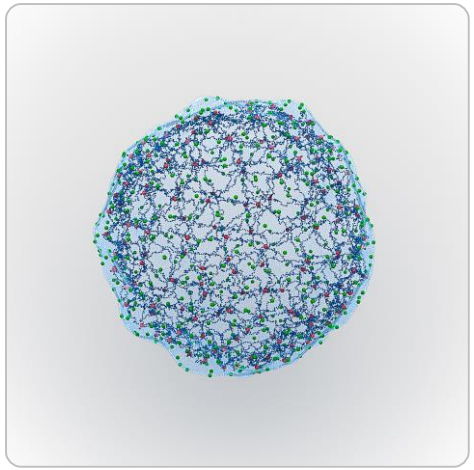
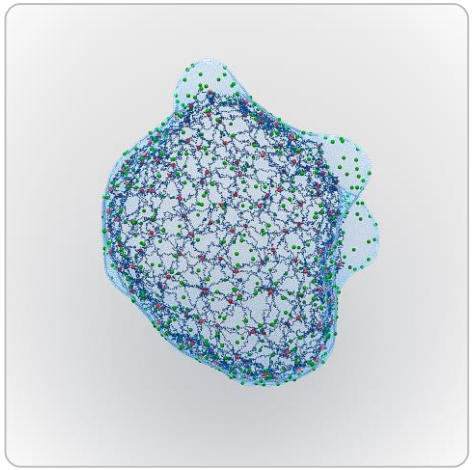
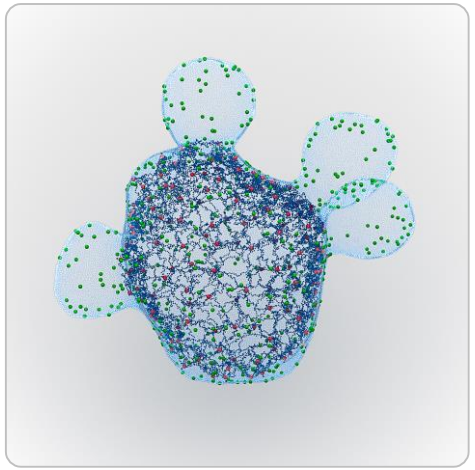
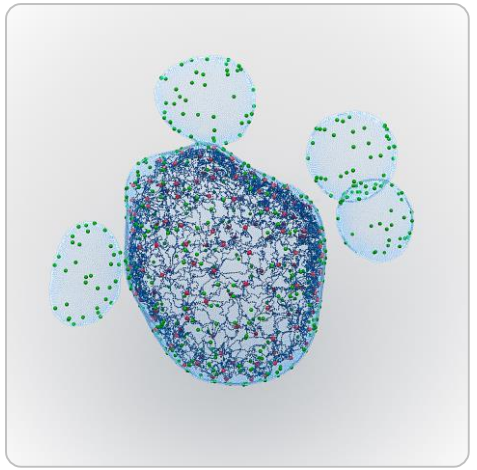
Validation & Summary

- Simulations of RBC vesiculation and membrane fluctuation
- Algorithm for Adaptive spatial search and load balancing
- 10x speedup, 40x bigger system
- Open-source at http://www.github.com/yhtang/OpenRBC

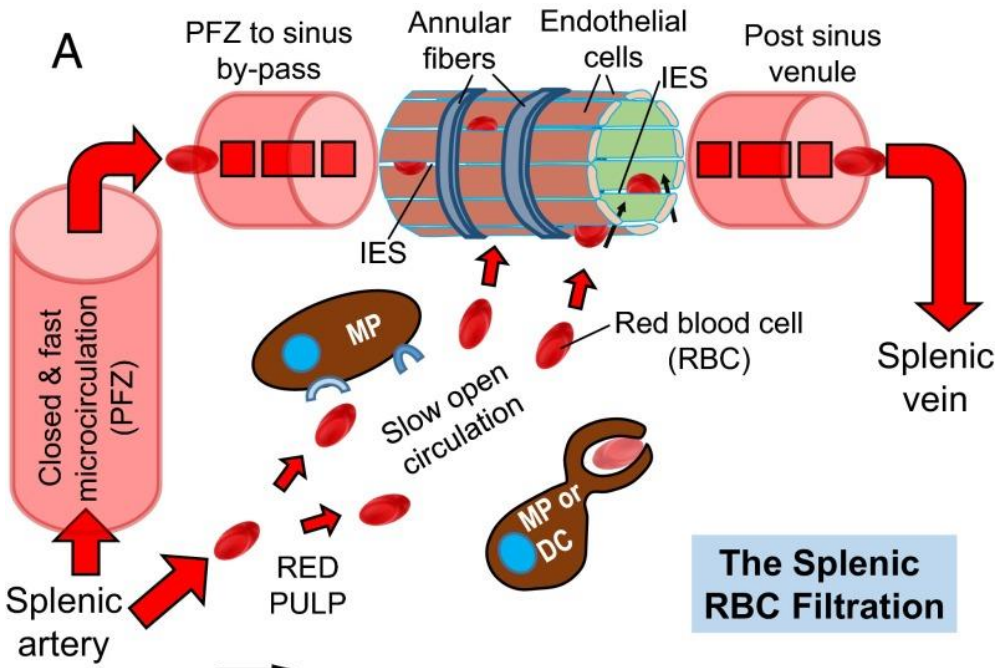


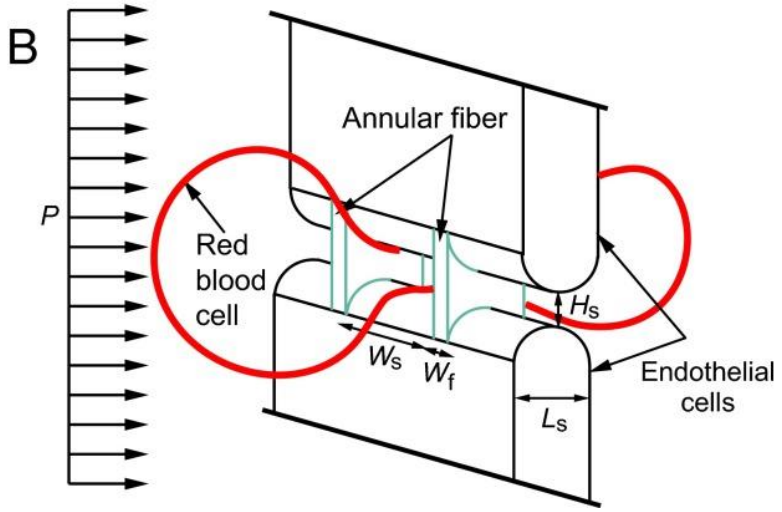
Capability & Design			
	OpenRBC	Legacy	Improvement
Problem size	>8×10^6	2×10^5	>40x
Line of Code	4677	7424	37% less

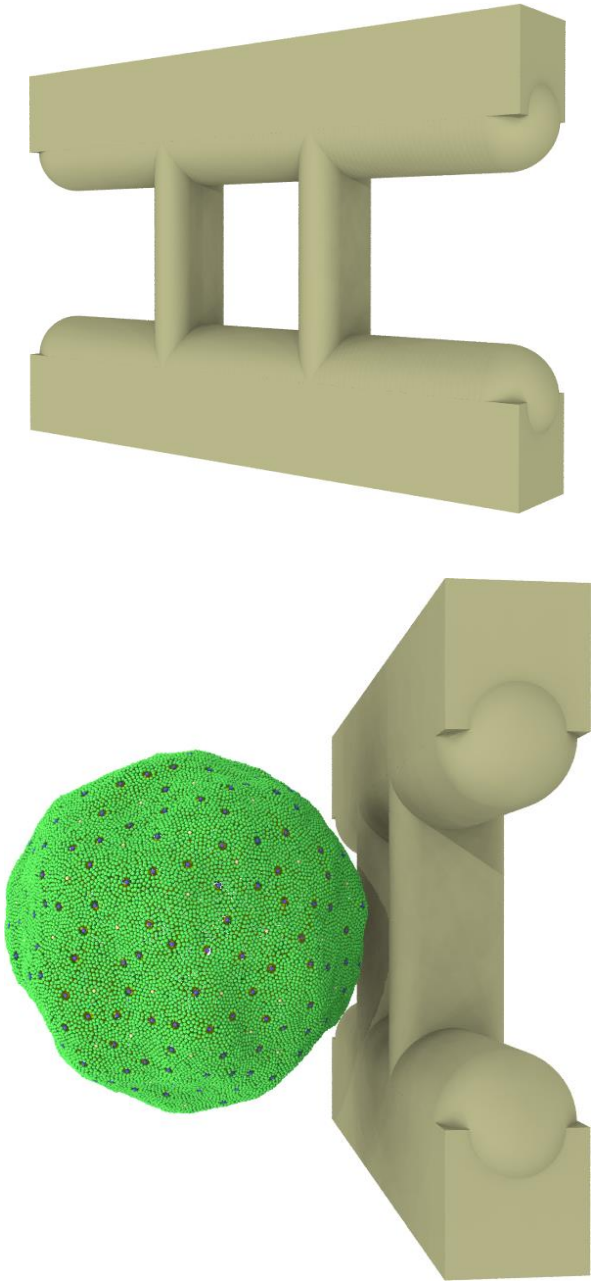
Performance – time steps/day				
Cores	Particles	OpenRBC	Legacy	Speedup
20	8.34×10^6	3.90×10^5	-	-
4	1.88×10^5	3.86×10^6	0.42×10^6	9.2x

Application: RBCs Pass through Spleen (Preliminary Results)

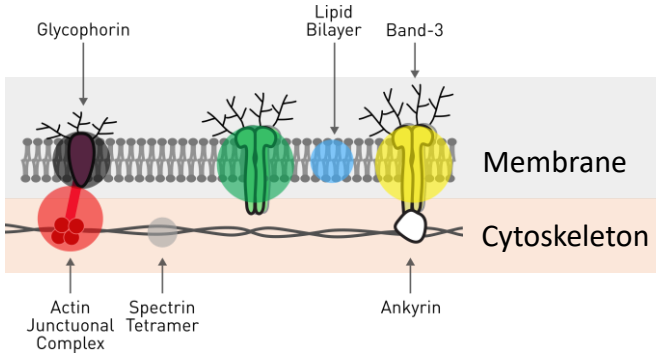




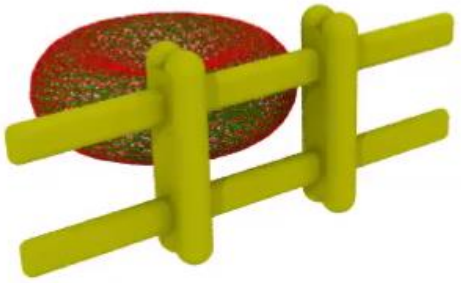


Pivkin, et al., *PNAS*, 2016.

Applications: RBCs Pass through Spleen (Preliminary Results)

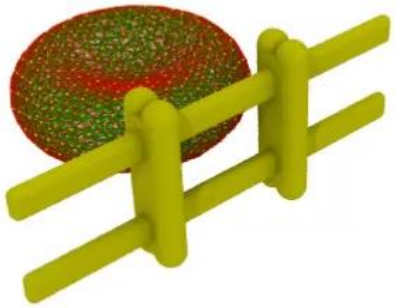


› Healthy RBC: pass

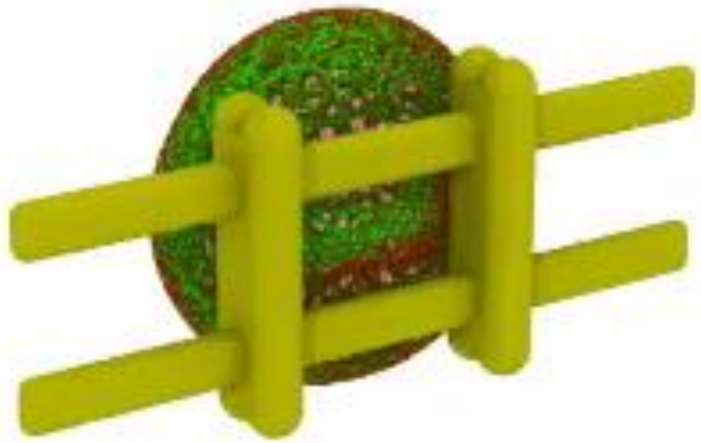


› #Actin-Glycophorin 20%: cell lysis

› #Band3-Spectrin 40%: vesiculation



› Spherical cell: stuck due to small S/V ratio



Thank you!

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Computing Resource

OLCF INCITE Project BIP017, BIP102, BIP118