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Human Arterial-Tree Multi-scale Modeling, Simulations and Visualization

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Human arterial-tree multi-scale simulations

- The human vascular system is incredibly complex, with 5 liters of blood traveling 60,000 miles in just 1 minute

The success of applying CFD as a truly predictive tool depends on the ability to accurately simulate the *blood flow at all spatial scales.*

For modeling purposes, we subdivide the arterial system into three levels:

1)The **Macrovascular** Network (*MaN*), which includes large arteries, down to a diameter of 0.5 mm

2)The **Mesovascular** Network (*MeN*), which includes small arteries and arterioles, from 500 μm down to 10 μm

3)The **Microvascular** Network (*MiN*), which represents the capillary bed

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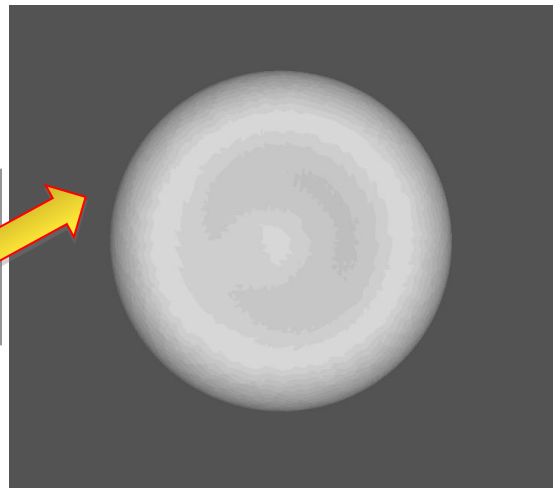
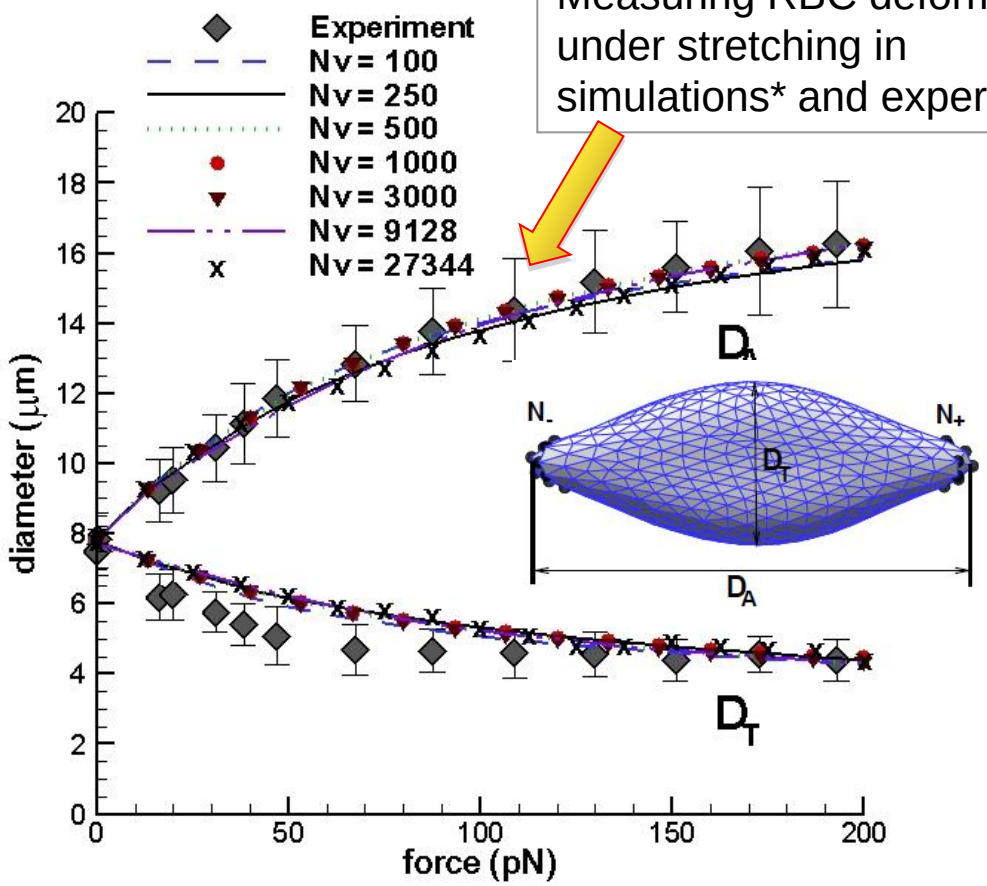
Atomistic modeling of blood cells: Validation

Measuring RBC deformation under stretching in simulations* and experiments**





The blood cell model* implemented in DPD-LAMMPS has been verified in experiments**. Each red blood cell is represented by O(100) DPD particles in order to obtain physiologically correct dynamics.

*Simulations: Fedosov et al., *Biophysical Journal*, 98(10):2215–2225, 2010.

**Experiment: - Suresh et al., *Acta Biomaterialia*, 1:15-30, 2005

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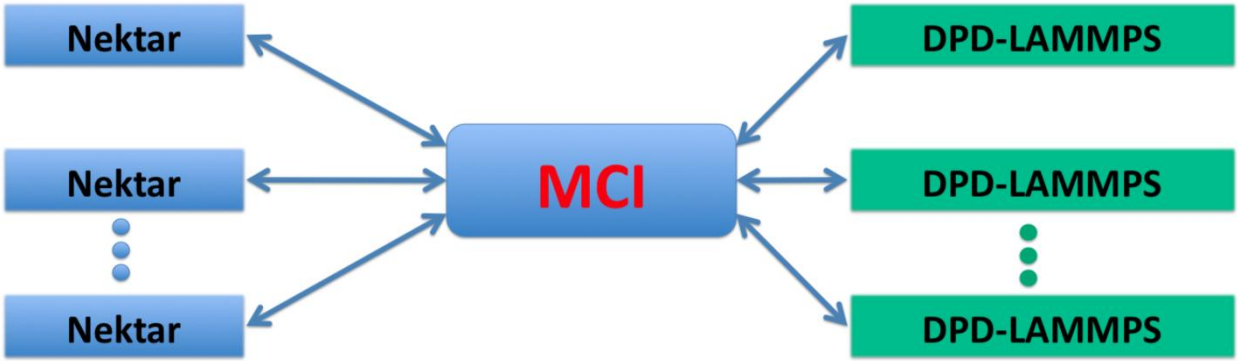
Multi-scale modeling of blood clot formation

- **We present the computational advances that have enabled multi-scale simulation of blood clot formation on 190,740 processors by coupling a high-order (spectral element) Navier-Stokes solver with a stochastic (coarse-grained) Molecular Dynamics solver based on Dissipative Particle Dynamics (DPD-LAMMPS)*.**



*L. Grinberg *et. al. A new computational paradigm in multi-scale simulations: Application to brain blood flow.* To be presented at *SC11,* ACM Gordon Bell Finalist.

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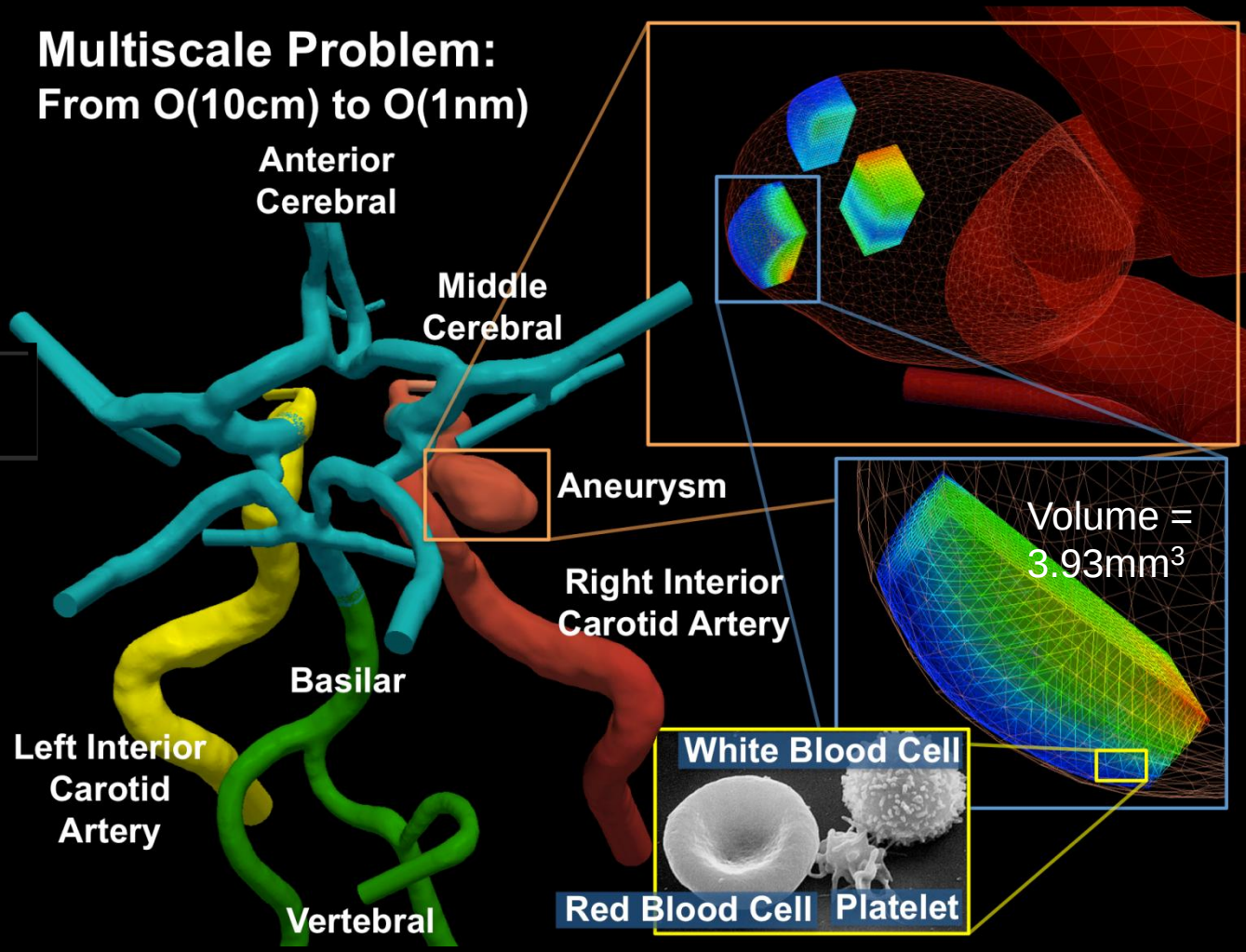
Coupled continuum-atomistic simulations

The macro-scale dynamics in the brain arterial network (about 3 billion unknowns) are resolved by *Nektar* - a spectral element solver.

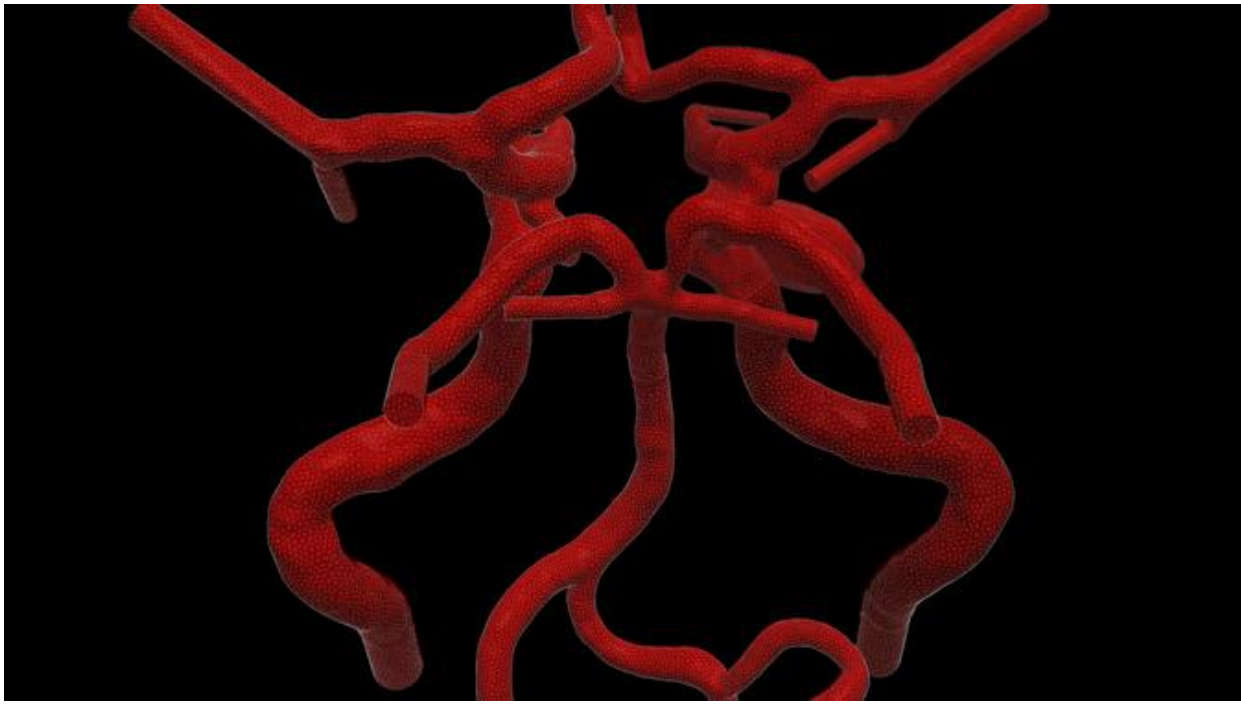
The micro-scale flow and cell dynamics within the aneurysm are resolved by an in-house version of DPD-LAMMPS (for an equivalent of about 100 billion molecules).

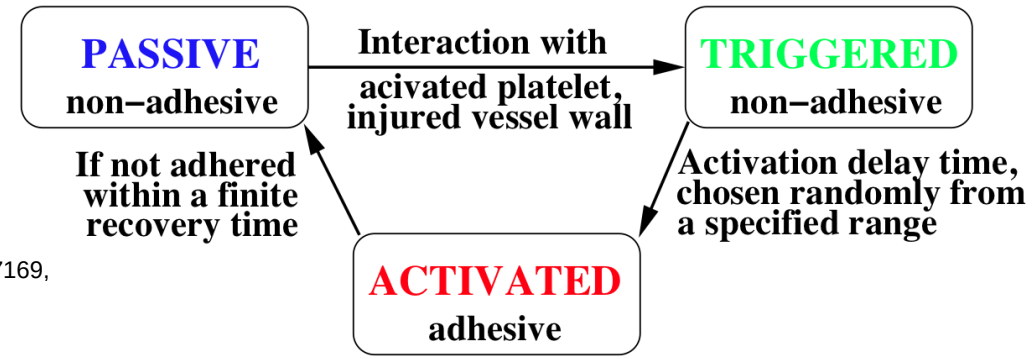
The two solvers are coupled through interface boundary conditions and communicate through a multi-level communicating interface.



Multi-scale modeling of blood clot formation

The animation shows:
1) Patient-specific geometry of brain vasculature with an aneurysm.
2) Streamlines inside the aneurysm depicting the large scale flow patterns.
3) A sub-region inside the aneurysm where atomistic solver has been applied for platelet aggregation simulation.
4) Platelets transition from a passive to active state and aggregation of platelets at the wall of the aneurysm*,**.





*P. Richardson and G. Born. *Activation time of blood platelets*. J. Membrane Biology, 57:87–90, 1980.

**I. V. Pivkin, P. D. Richardson, and G. E. Karniadakis. *Blood flow velocity effects and role of activation delay time on growth and form of platelet thrombi*. PNAS USA, 103(46):17164–17169, 2006

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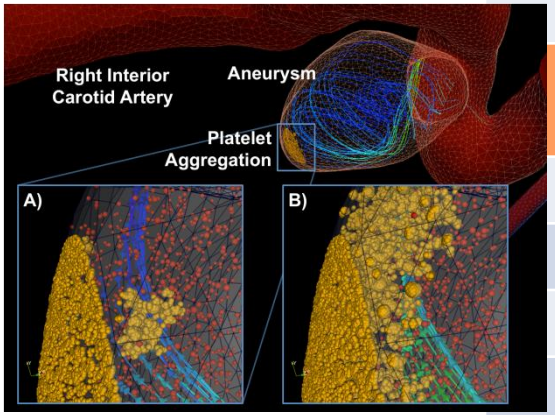
Coupled continuum-atomistic solver: Scaling

Ncore (DPD-LAMMPS+Nektar)	CPU-time [s]	efficiency
	BlueGene/P (ANL)	
28,672 + 4,096	3506	reference
61,440 + 4,096	1400	1.07
126,976 + 4,096	666	1.02
	CRAY XT5 (NICS, ORNL)	
17,280 + 4,116	2194	reference
25,920 + 4,116	1177	1.24
34,560 + 4,116	763 (806)	1.15
93,312 + 4,116	226 (280)	1.25 (1.07)
186,624 + 4,116	(206)	(0.68)



Blood clot formation. Yellow spheres represent activated platelets

Continuum domain: 425K spectral elements (1B d.o.f with P=6; 3.2B d.o.f with P=10)

Atomistic domain: 823,079,981 DPD particles

CPU time for 200 Nektar's (4,000 DPD-LAMMPS) time-steps + I/O

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Computations were performed on the CRAY XT5 of NICS and ORNL, and BlueGene/P of ANL

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