

# TACC SITE UPDATE

The background is a dark blue gradient with glowing orange circuit lines and geometric shapes. On the right side, there is a stylized, low-poly illustration of a person in a white shirt and orange vest, holding a glowing blue object, standing on a rocky, orange terrain.

**Tommy Minyard**

Frontera Co-PI and Chief Systems Engineer  
Director of Advanced Computing Systems  
Texas Advanced Computing Center

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# STAMPEDE2

- ▶ Workhorse Supercomputer with 4,200 KNL and 1,736 SKX nodes
- ▶ Supports the broad science mission at NSF and part of XSEDE
- ▶ Almost 1000 projects have had allocations on the system
- ▶ Over 4.5 million jobs ranging from single node all the way up to full system runs across both KNL and SKX nodes

# FRONTERA COMPUTE NODES

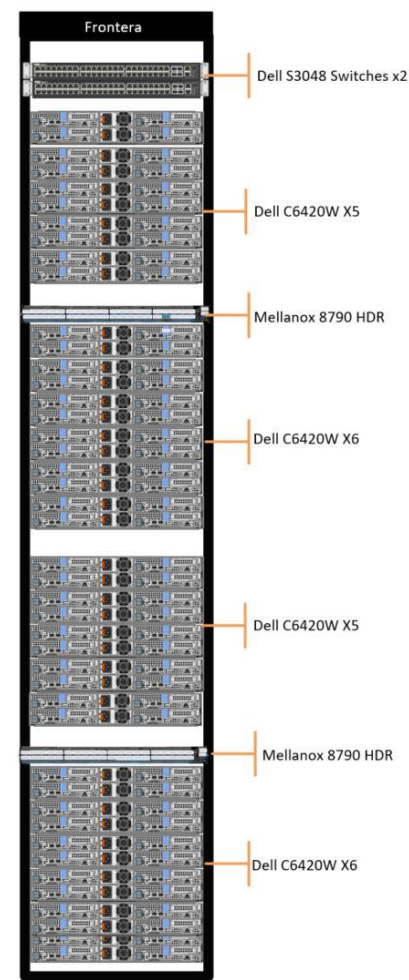
- ▶ 2,002 Dell C6420 chassis, 4 nodes per chassis
  - ▶ 8,008 total compute nodes
    - ▶ Two Intel “Cascade Lake” (CLX) Xeon Platinum 8280 CPUs
      - ▶ 28 cores per socket, 205W TDP
      - ▶ Nominal frequency of 2.7GHz, 2.4 Tflops
    - ▶ 192 GB (12x16GB) 2933MHz DDR4
    - ▶ 240 GB SSD
    - ▶ Mellanox ConnectX-6 HDR100 InfiniBand (IB) PCIe card
    - ▶ Integrated iDRAC management
    - ▶ Cool-IT liquid cooling to the processors
  - ▶ Redundant 2400W power supplies



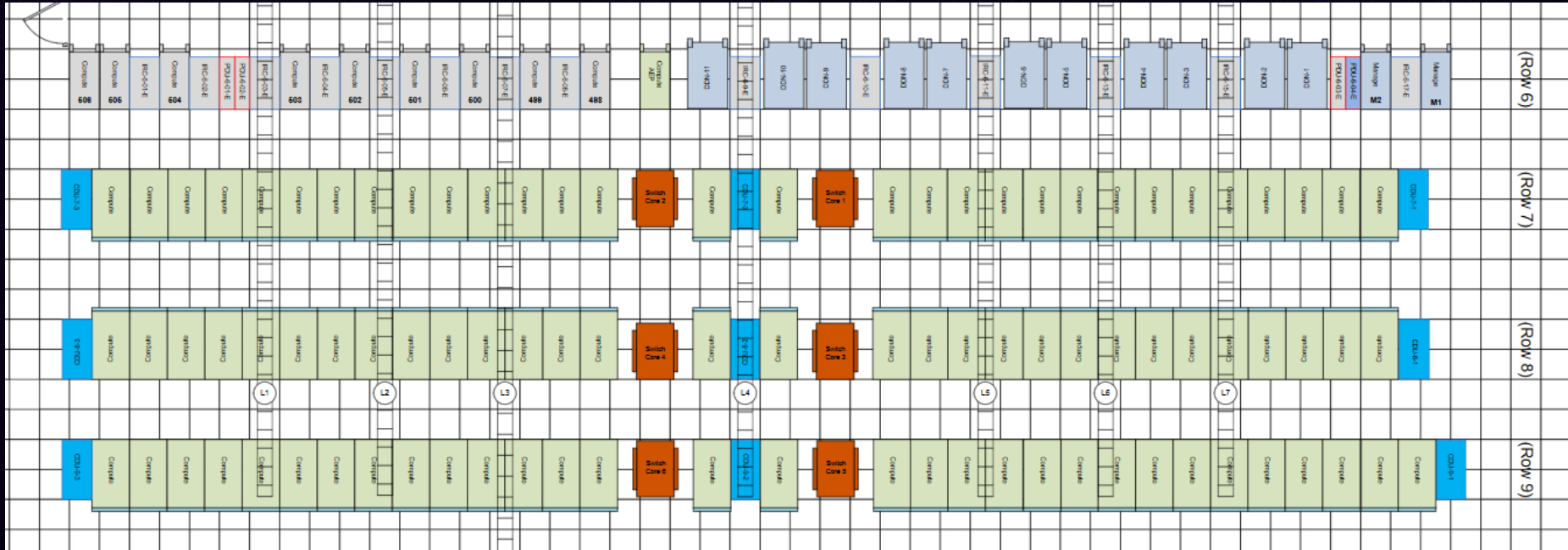


# COMPUTE RACK LAYOUT

- ▶ 54U, 750mm wide racks, 91 total racks
- ▶ Layout design based on IB switch port count
- ▶ 22 chassis / 88 nodes per rack in two groups
- ▶ Two Mellanox HDR 40-port switches
  - ▶ 44 nodes at 100Gbps, 18 uplinks at 200Gbps
- ▶ Two 48-port GigE switches
- ▶ Liquid cooling manifolds
- ▶ Cool doors for supplemental cooling
- ▶ Rack cabling routed to allow for hot-swap of components



# FRONTERA LAYOUT



# SYSTEM CONSTRUCTION COMPLETE

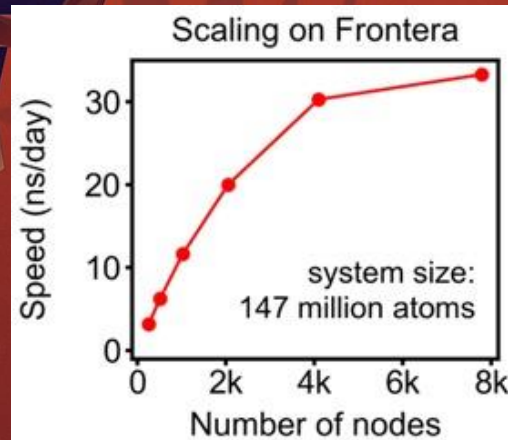
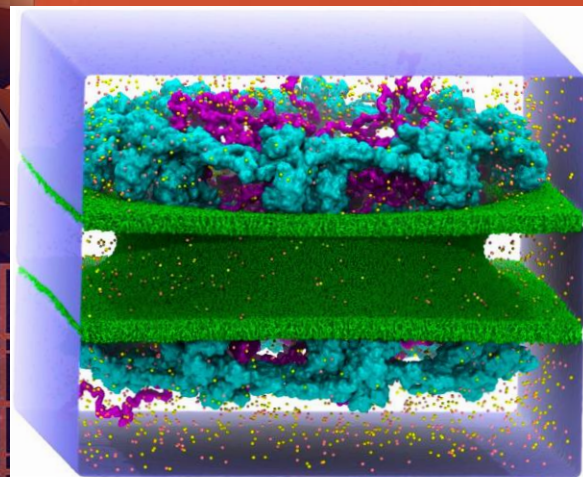




# CENTER FOR THE PHYSICS OF LIVING CELLS

ALEKSEI AKSIMENTIEV  
UNIVERSITY OF ILLINOIS AT URBANA-  
CHAMPAIGN

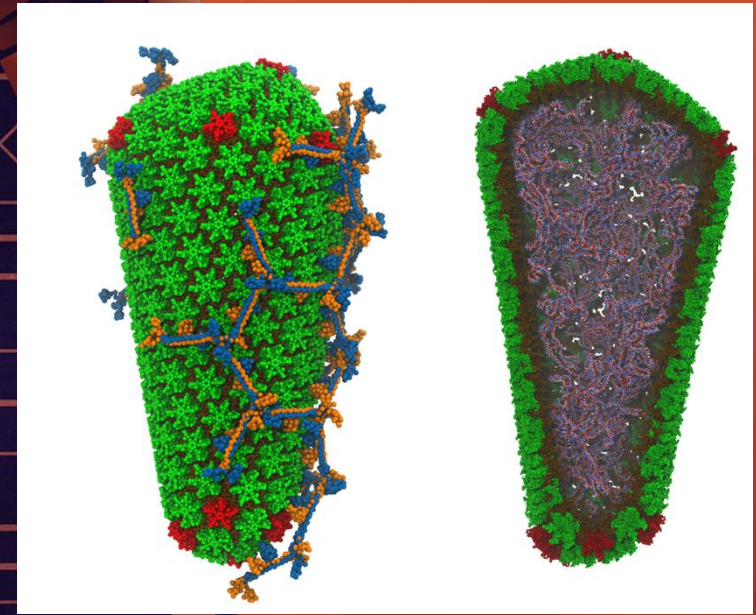
- The nuclear pore complex serves as a gatekeeper, regulating the transport of biomolecules in and out of the nucleus of a biological cell.
- To uncover the mechanism of such selective transport, the Aksimentiev lab at UIUC constructed a computational model of the complex.
- The team simulated the model using memory-optimized NAMD 2.13, 8tasks/node, MPI+SMP.
- Ran on up to 7,780 nodes on Frontera.
- One of the largest biomolecular simulations ever performed.
- Scaled close to linear on up to half of the machine.
- Plan to build a new system twice as large to take advantage of large runs



# FRONTIERS OF COARSE-GRAINING

GREGORY VOTH  
UNIVERSITY OF CHICAGO

- Mature HIV-1 capsid proteins self-assemble into large fullerene-cone structures.
- These capsids enclose the infective genetic material of the virus and transport viral DNA from virion particles into the nucleus of newly infected cells.
- On Frontera, Voth's team simulated a viral capsid containing RNA and stabilizing cellular factors in full atomic detail for over 500 ns.
- First molecular simulations of HIV capsids that contain biological components of the virus within the capsid.
- The team ran on 4,000 nodes on Frontera.
- Measured the response of the capsid to molecular components such as including genetic cargo and cellular factors that affect the stability of the capsid.



"State-of-the-art supercomputing resources like Frontera are an invaluable resource for researchers. Molecular processes that determine the chemistry of life are often interconnected and difficult to probe in isolation. Frontera enables large-scale simulations that examine these processes, and this type of science simply cannot be performed on smaller supercomputing resources."

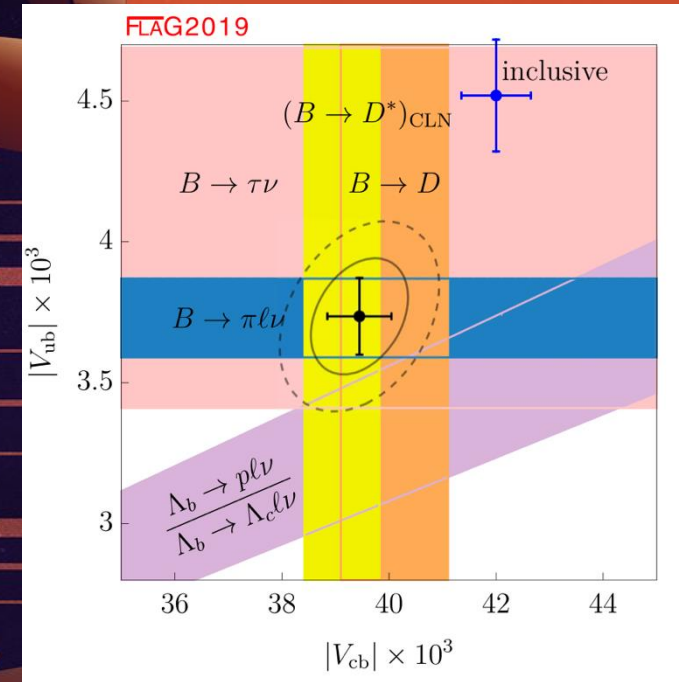
-Alvin Yu, Postdoctoral Scholar in Voth Group



# LATTICE GAUGE THEORY AT THE INTENSITY FRONTIER

CARLTON DETAR  
UNIVERSITY OF UTAH

- Ab initio numerical simulations of quantum chromodynamics (QCD) help obtain precise predictions for the strong-interaction environment of the decays of mesons that contain a heavy bottom quark.
- Compare predictions with results of experimental measurements to look for discrepancies that point the way to new fundamental particles and interactions.
- Carried out the very initial steps in the shuffle for the Exascale-size lattice during Frontera large-scale capability demonstration.
- 16x larger problem than anything they had previously calculated.
- Ran on 3,400+ nodes.
- The capability demonstration showed that given sufficient resources the team can run an Exascale-level calculation on Frontera.



"In addition to demonstrating feasibility, we obtained a useful result. We are now in good position for a future exascale run. We have working code and a working starting gauge configuration file."

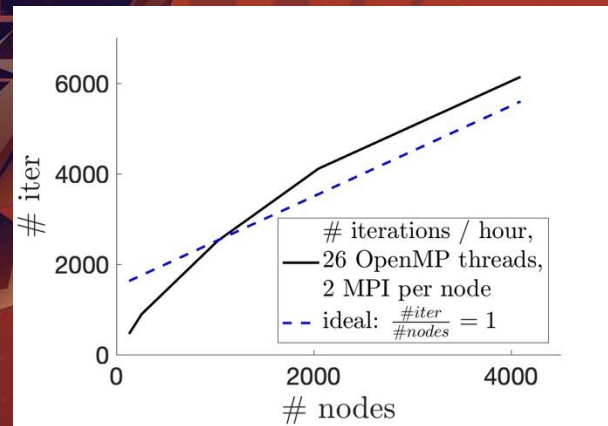
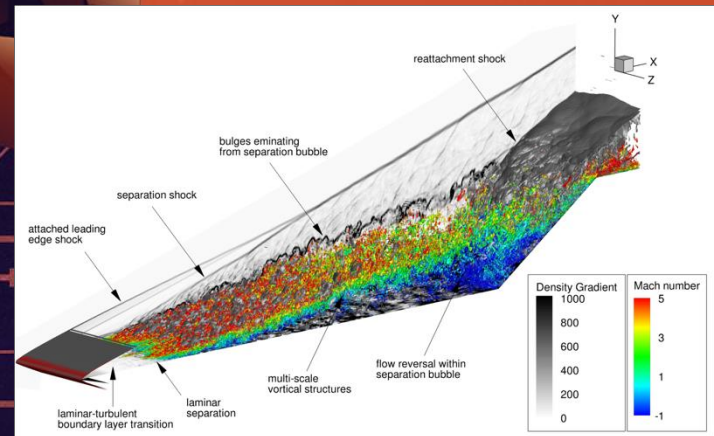
- Carlton DeTar, University of Utah

# PREDICTION AND CONTROL OF TURBULENCE-GENERATED SOUND

DANIEL BODONY

UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

- Simulated fluid-structure interactions relevant to hypersonic vehicles.
- Simulations replicated a companion experiment performed at NASA Langley in their 20-inch Mach 6 tunnel.
- Frontera runs used 2 MPI ranks per node (one per socket) and 26 OpenMP threads per MPI rank.
- Saw superlinear speedup on up to 2,000+ nodes by fitting into cache rather than fetching from main memory.
- Linear speedup up to 4,000 nodes.

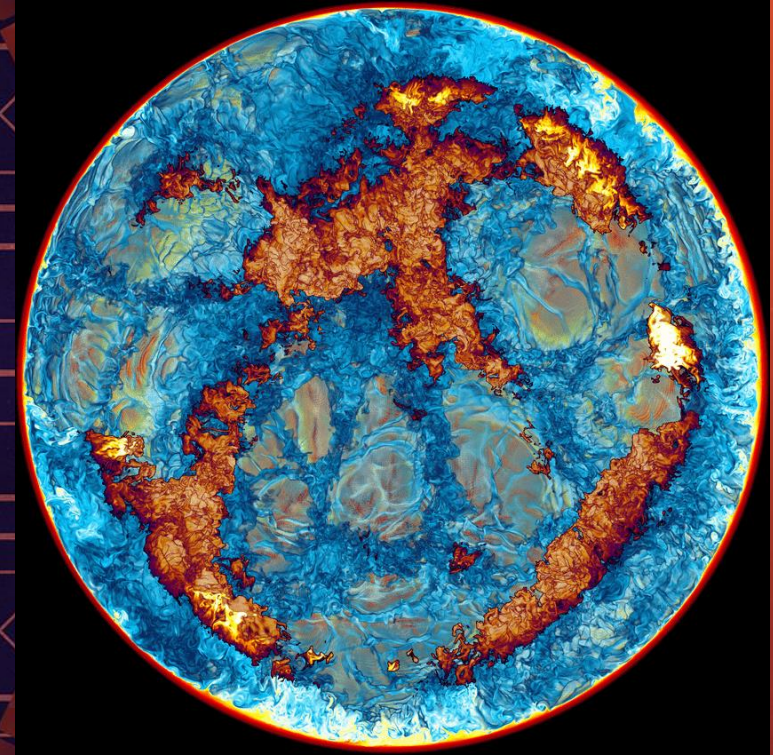




# 3-D STELLAR HYDRODYNAMICS

PAUL WOODWARD  
UNIVERSITY OF MINNESOTA

- The project's goal is to study the process of Convective Boundary Mixing (CBM) and shell mergers in massive stars.
- The computational plan includes a sequence of brief three-dimensional simulations alternating with longer one-dimensional simulations.
- Ran on 7,300+ nodes for more than 80 hours during Frontera large-scale capability demonstration.
- Saw 588 GFlop/s/node — or 4 Petaflops of sustained performance — for more than 3 days!





# SUMMARY

- ▶ Challenging deployment due to compressed schedule
- ▶ Higher than anticipated technical issues, but not atypical of new system deployments
- ▶ Early user operation demonstrated system stable for users
- ▶ Performance and stability continuing to improve with evolving firmware and updated software libraries
- ▶ Full system jobs running smoothly and reliably



# FRONTERA

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