EXAMPLES OF AI/ML ENABLED BY HPC APPLIED TO A QIS

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Motivations for QIS based on a Storage Ring

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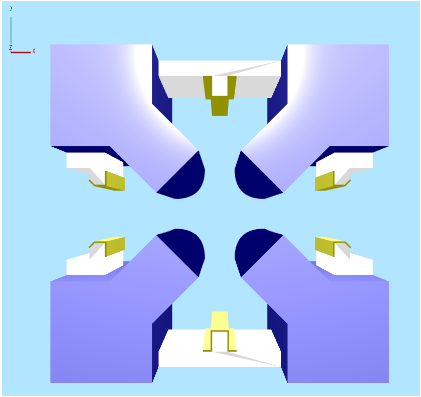
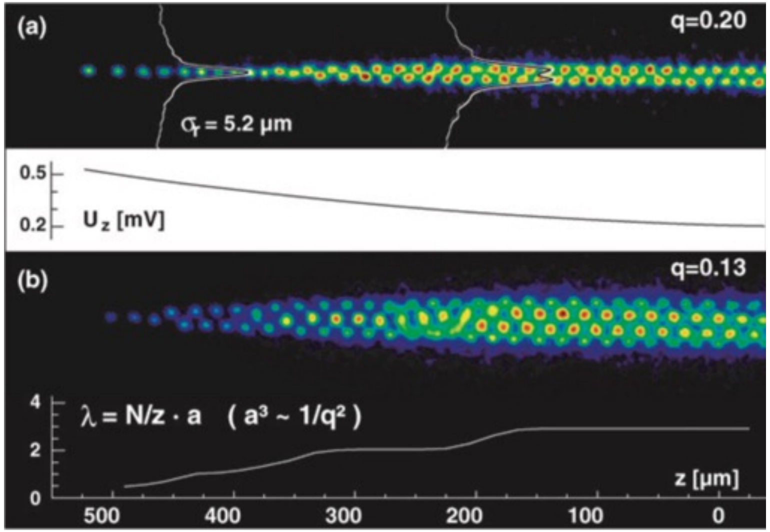


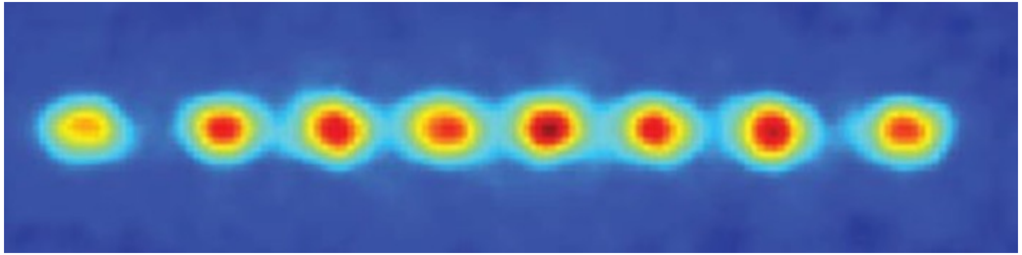
- Modern ion traps contain a few hundred ions at most.
- A Storage Ring can already “trap” orders of magnitude more ions.
- The key is the laser cooling of the ion beam in the storage ring
  - Crystalline beam and Ion Coulomb Crystal formation.
  - Access to the quantum states of individual ions.
- An ICC trapped in SRQC could potentially contain thousands of ions.
  - Multiple long ICCs held in different RF buckets.
  - Could also run multiple and separate quantum computations.
- Here we address the calculation of the equilibrium state of an ICC in a new regime of number of ions.
  - A SRQC system should be able to “reset” itself to the base state after performing a computation.

Crystalline Beams in Storage Rings



U. Schramm, T. Schätz, M Bussmann and D. Habs
Plasma Phys. Control. Fusion **44** (2002) B375–B387

Sektion Physik, LMU München, D-85748 Garching, Germany



Christopher R. Monroe and David J. Wineland

- By using beam cooling techniques, ion beam temperatures can be reduced to the point that repelling Coulomb forces balance against external forces.
- Two states can be created:
  - Crystalline beam.
  - Ion Coulomb Crystal

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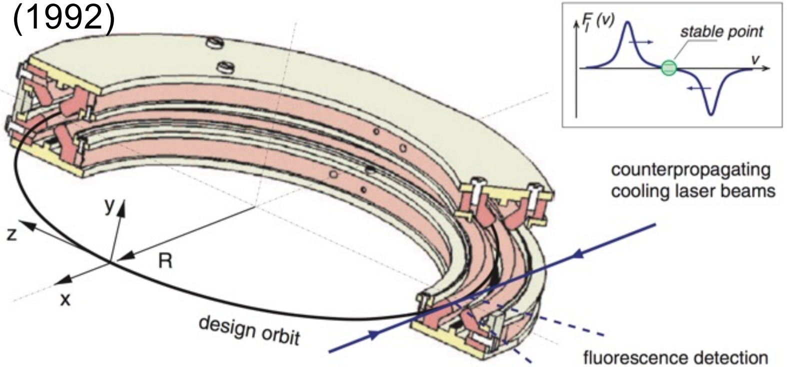
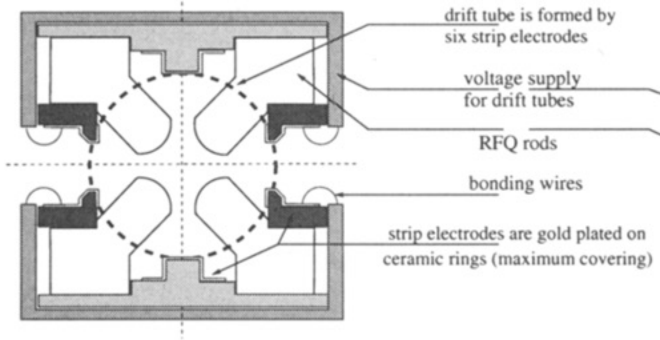
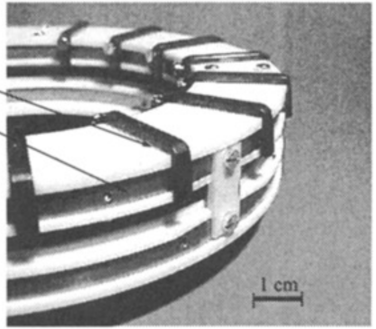
PALLAS RF-Quadrupole Ring Trap

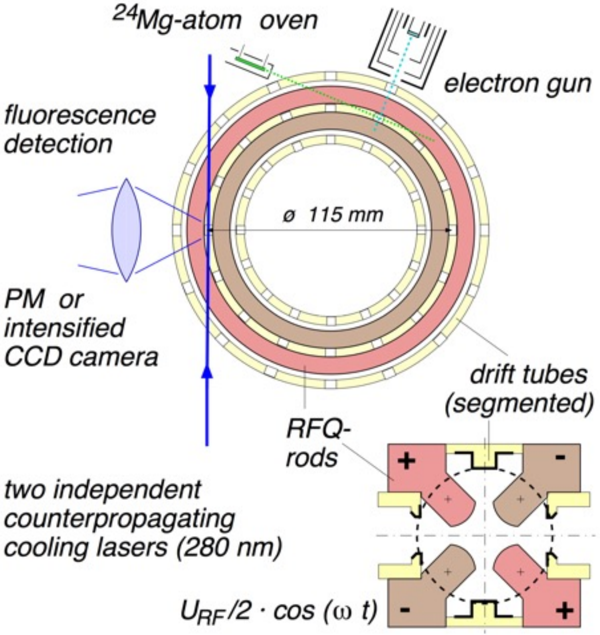
Multiple-shell structures of laser-cooled 24Mg+ ions in a quadrupole storage ring G. Birkl, S. Kassner, H. Walther: Nature **357**, 310 (1992)

U Schramm1, T Schätz, M Bussmann and D Habs
Sektion Physik, Ludwig-Maximilians-Universität München, D-85748 Garching, Germany

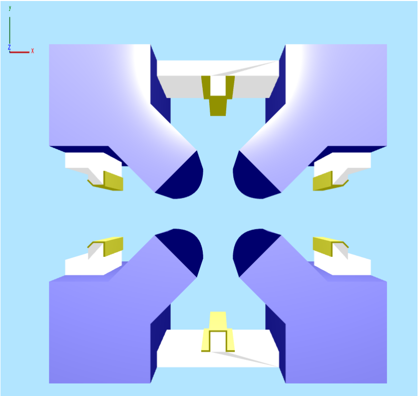


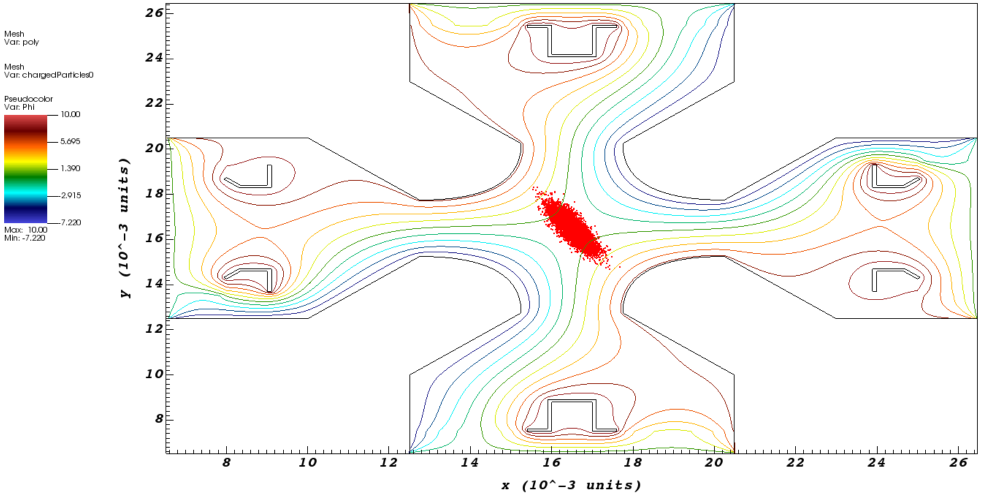






EM design of a CRFQ for QIS





- EM and beam dynamics using VSim.
- Beam stability over time ensures sufficient cooling time to crystalline state.
- Design considerations include:
  - Pipe opening for laser cooling.
  - Control rods.

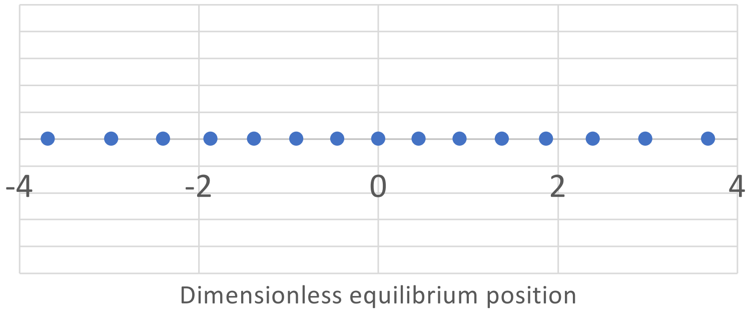
VSim
https://txcorp.com/vsim/

The system: A 1D ion trap

- Ions are bounded to 1D by the trap rf fields.
- The potential energy of the 1D system is:

$$V = \sum_{m=1}^{N} \frac{1}{2} M\nu^2 x_m(t)^2 + \sum_{m\neq n}^{N} \frac{Z^2e^2}{8\pi\varepsilon_0} \frac{1}{|x_n(t) - x_m(t)|}$$

Ion chain for N=15



- The **equilibrium positions** of the *N* ions in the chain are solved from:

$$u_m - \sum_{n=1}^{m-1} \frac{1}{(u_m - u_n)^2} + \sum_{n=m+1}^{N} \frac{1}{(u_m - u_n)^2} = 0\,; \quad m = 1, 2, \dots, N.$$

  – A function of the number of ions *N*.

  – A system of *N* coupled non-linear algebraic equations.

D.F.V. James, Appl. Phys. B 66, 181-190 (1998)

Numerical solution of the 1D equilibrium

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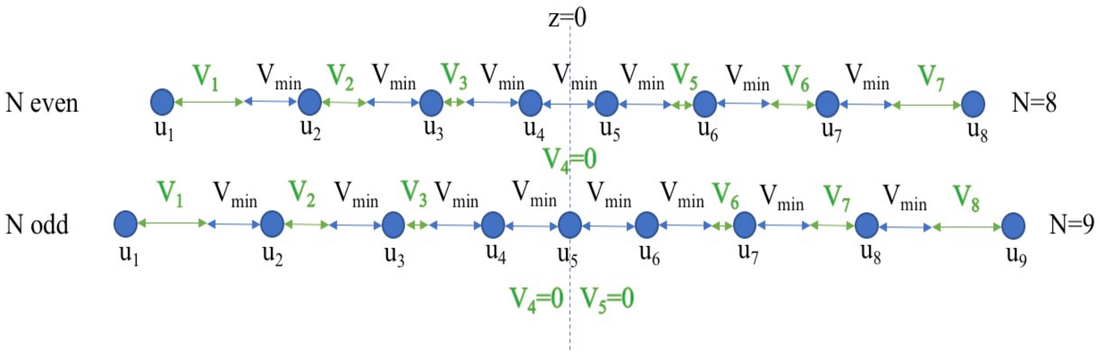
- This problem can be solved using readily available numerical libraries.
- For N>>1, the numerical calculation quickly becomes computationally expensive.
- This problem can be formulated in terms of the minimum separation between ion.
  - This reduces the numbers of variables.

Table 1. Scaled equilibrium positions of the trapped ions for different total numbers of ions [a]

N	Scaled equilibrium positions									
2	−0.62996	0.62996								
3	−1.0772	0	1.0772							
4	−1.4368	−0.45438	0.45438	1.4368						
5	−1.7429	−0.8221	0	0.8221	1.7429					
6	−2.0123	−1.1361	−0.36992	0.36992	1.1361	2.0123				
7	−2.2545	−1.4129	−0.68694	0	0.68694	1.4129	2.2545			
8	−2.4758	−1.6621	−0.96701	−0.31802	0.31802	0.96701	1.6621	2.4758		
9	−2.6803	−1.8897	−1.2195	−0.59958	0	0.59958	1.2195	1.8897	2.6803	
10	−2.8708	−2.10003	−1.4504	−0.85378	−0.2821	0.2821	0.85378	1.4504	2.10003	2.8708

D.F.V. James, Appl. Phys. B 66, 181-190 (1998)



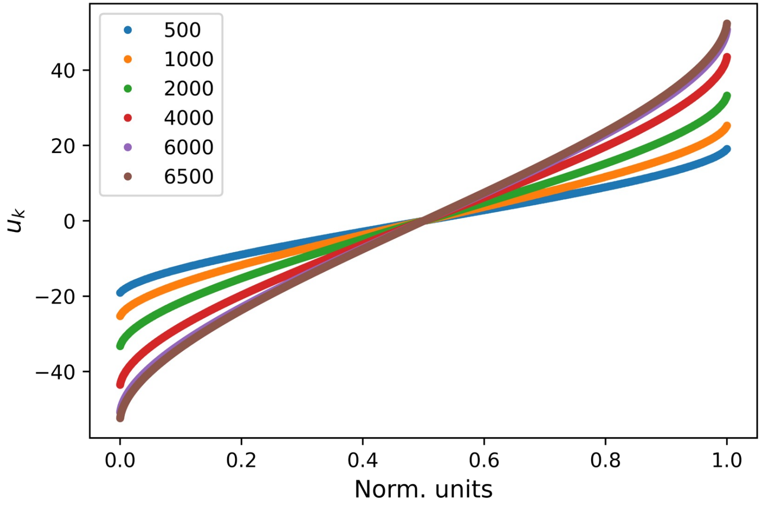
Courtesy of K. Brown and B. Huang.

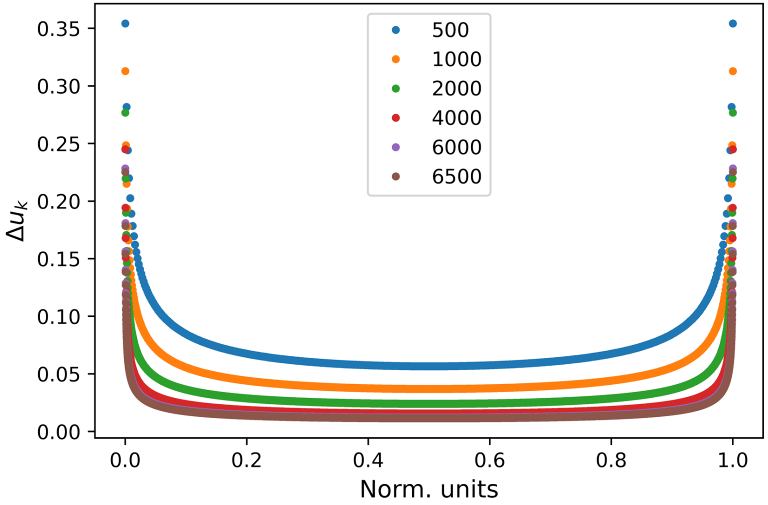
Numerical solution of the 1D equilibrium

- The **equilibrium positions** of the *N* ions in the chain are solved from:

$$u_m - \sum_{n=1}^{m-1} \frac{1}{(u_m - u_n)^2} + \sum_{n=m+1}^{N} \frac{1}{(u_m - u_n)^2} = 0\,; \quad m = 1, 2, \dots, N.$$

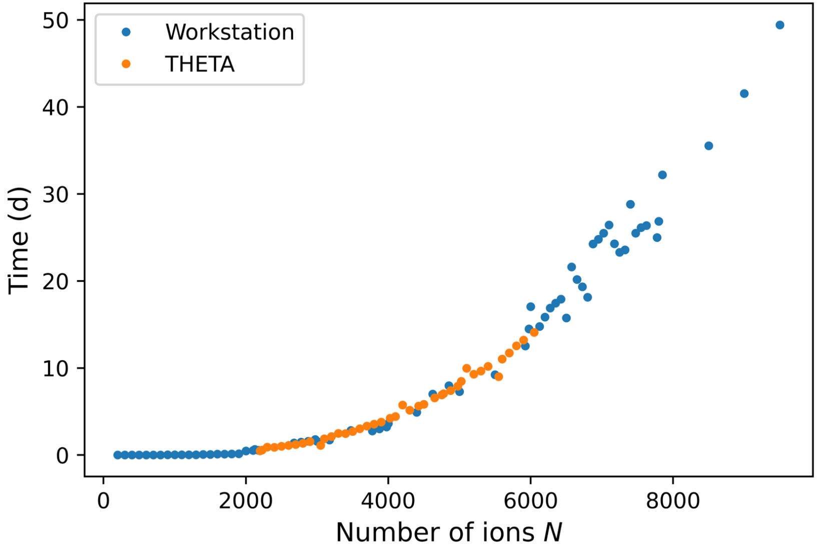
- Solution for different values of N:





Motivation for ML algorithms

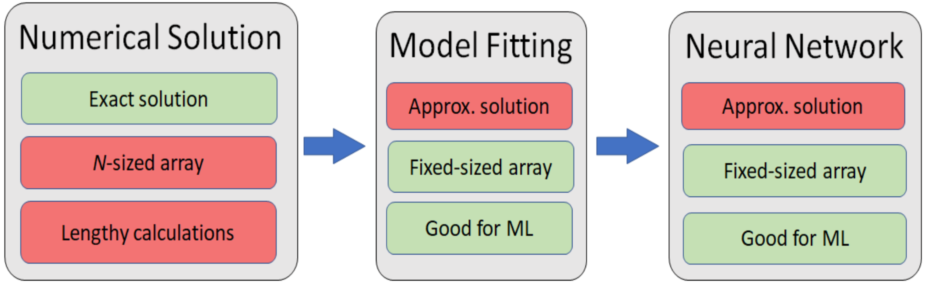
- The numerical calculation quickly becomes computationally expensive for large *N*.

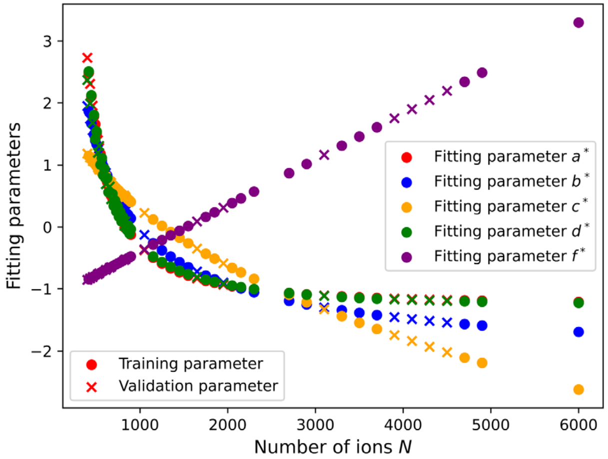


- Here we identify an opportunity to implement **ML algorithms for rapid calculation** *in lieu* of numerical calculation.

Rapid calculation of the equilibrium state with NN

- Approximate the solution given a discrete number of numerical solutions.





- Train a NN to predict the fitting parameters for solutions that have not been determined numerically.
- Reduced computation time at the cost of an approximation error.

Use an approximated model with a few fitting parameters. Train NN on the fitting parameters.

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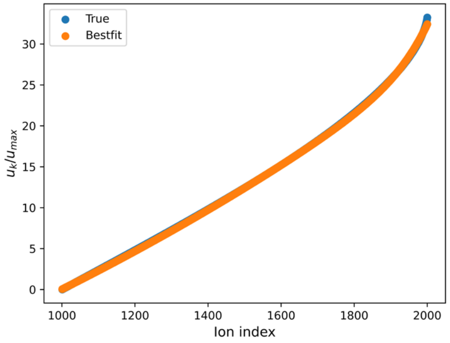
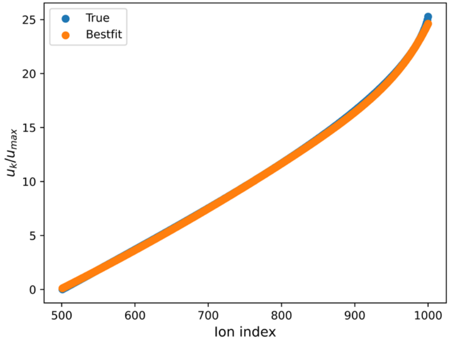
B. Huang *et al.*, in *IEEE Access*, vol. 10, 2022, doi: 10.1109/ACCESS.2022.3147727.

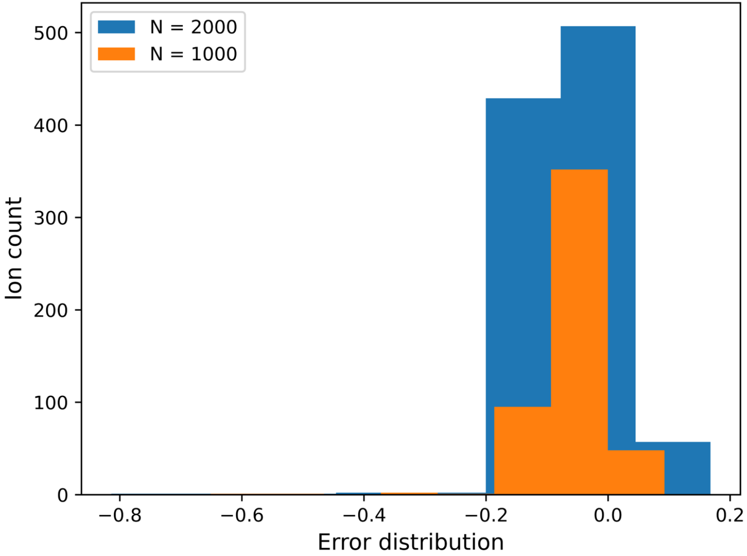
Prediction examples



Prediction of N=1000.



Prediction of N=2000.



Prediction error distribution, N=1000,2000.

THETA @ Argonne Leadership Computer Facility

- THETA is a 11.69 petaflops system based on the second-generation Intel® Xeon Phi™ processor, **281,088 cores.**

- General THETA architecture:
  - Theta has 4392 (KNL) nodes.
  - Each node has 64 physical cores.
  - Each core has 4 hardware threads.

- We currently use THETA for:
  - Electromagnetic simulations with VSim.
  - Optimization
  - AI, ML, DL, Surrogate models, etc.

Argonne NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY

THETA is the current ALCF flagship supercomputer.
https://www.alcf.anl.gov/theta

Other examples of work at ALCF

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Pankaj Rajak, Nitish Baradwaj, Ken-ichi Nomura, Aravind Krishnamoorthy, Jose P. Rino, Kohei Shimamura, Shogo Fukushima, Fuyuki Shimojo, Rajiv Kalia, Aiichiro Nakano, and Priya Vashishta*

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- This research also used computing resources from Element Aero.

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