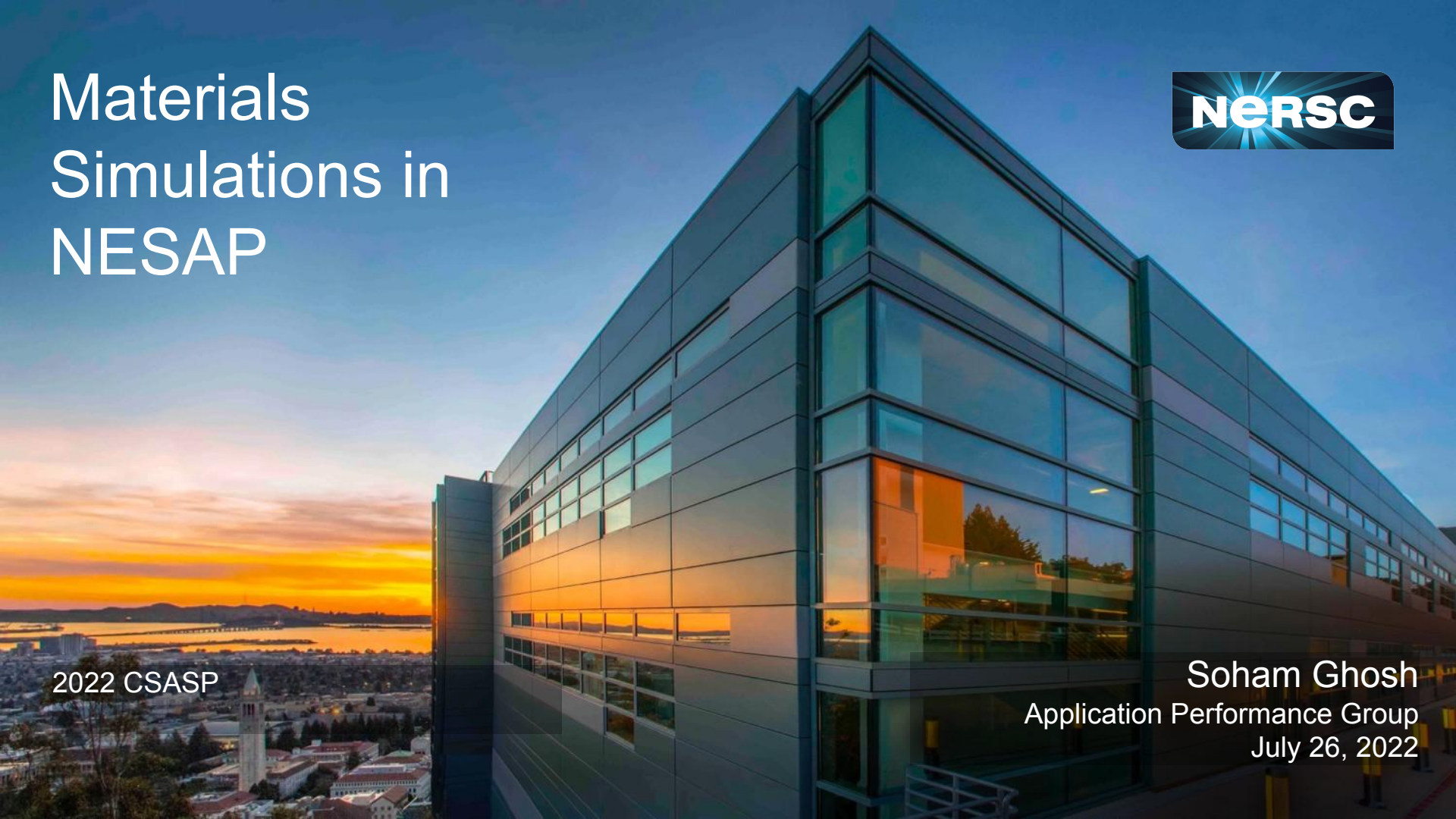
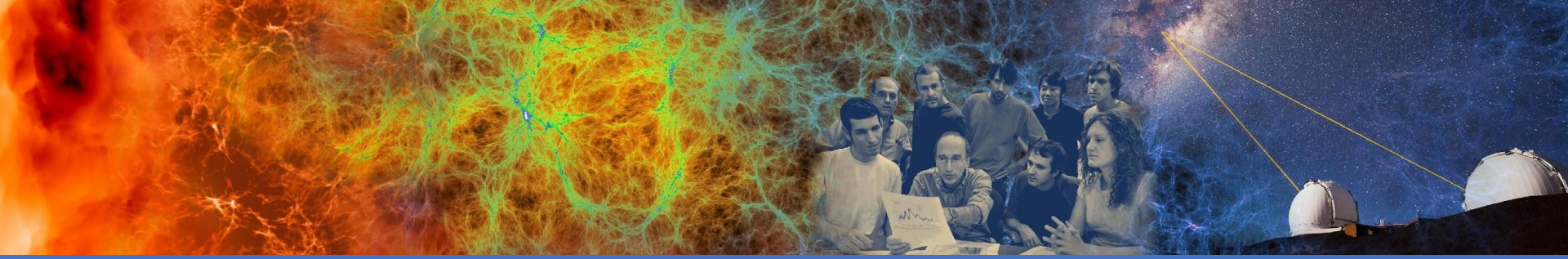
Materials Simulations in NESAP



2022 CSASP

Soham Ghosh
Application Performance Group
July 26, 2022

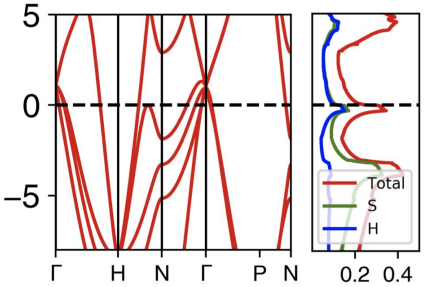


Materials simulations: Overview

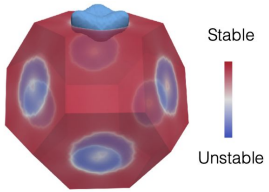
- What we do
- DFT, GW, ML
- Computational challenges
- Programming models

Simulation: What can it do?

bulk bands and dos

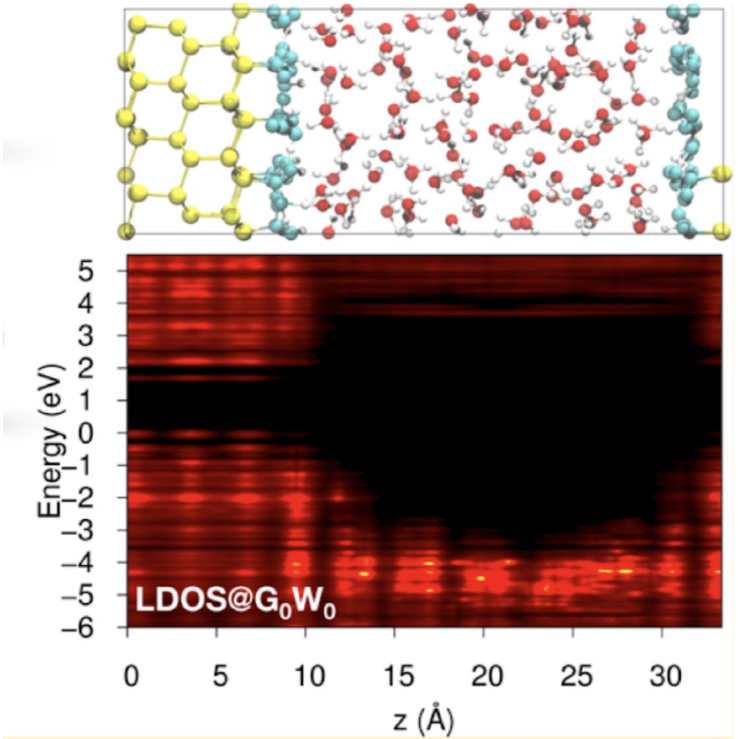


Phonon stability

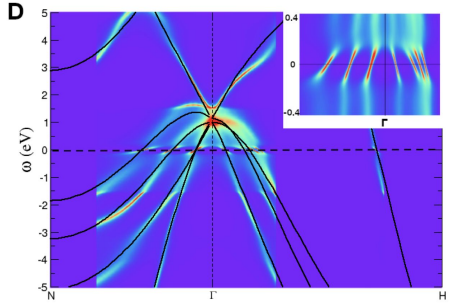


LaH_{10}

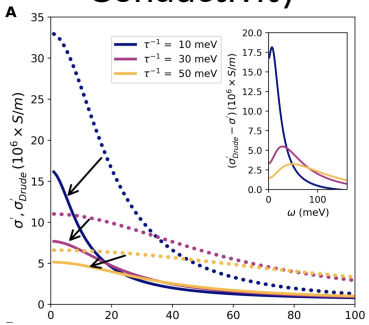
GW LDOS



El-ph interaction



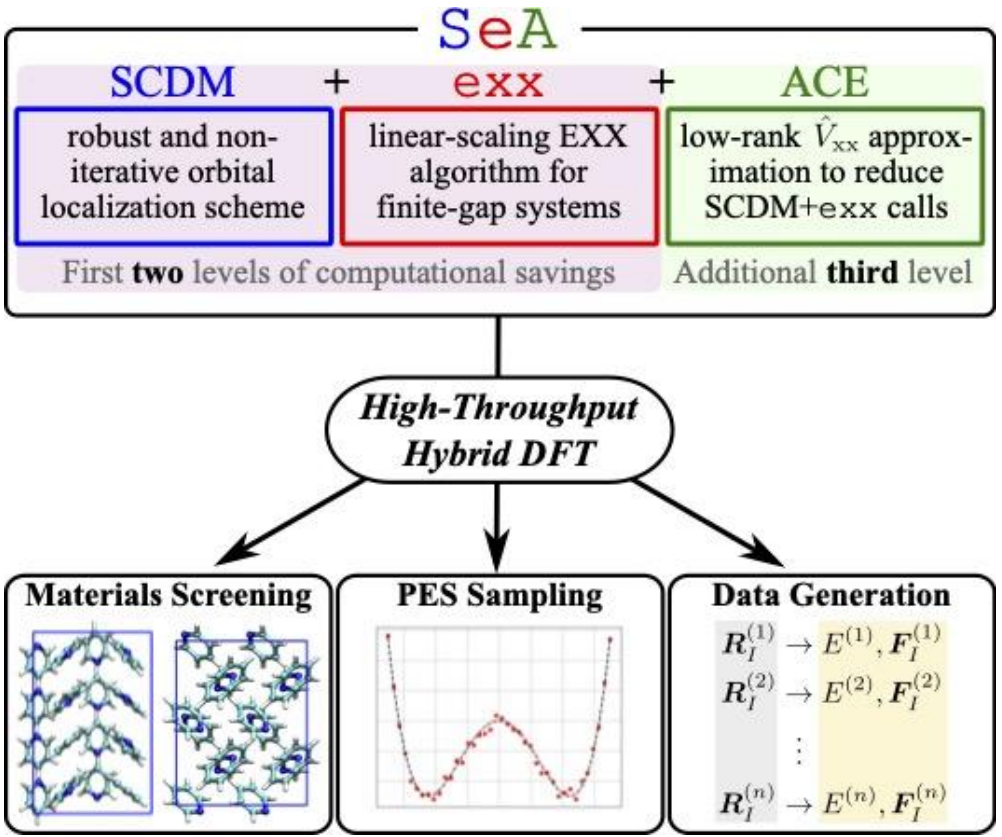
Conductivity



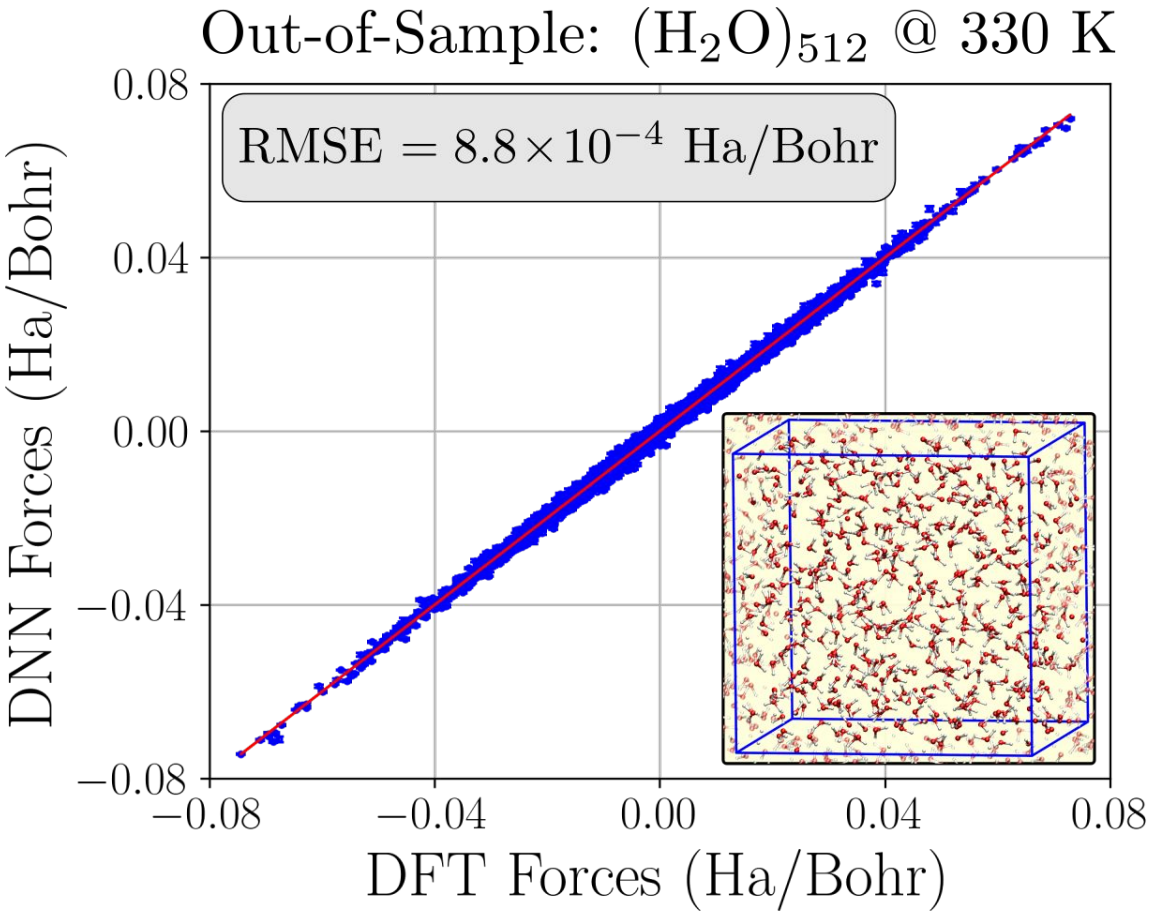
SSG, YX, ZM, EM, PRB(2016) YQ, SSG, WEP PRB (2019), MG and JG JCTC (2015)

QE: High-Throughput DFT

- Fortran-based
- MPI+openMP+libraries
- CUDA, cuBLAS, cuLAPACK
- OpenACC
- CUDA-aware MPI



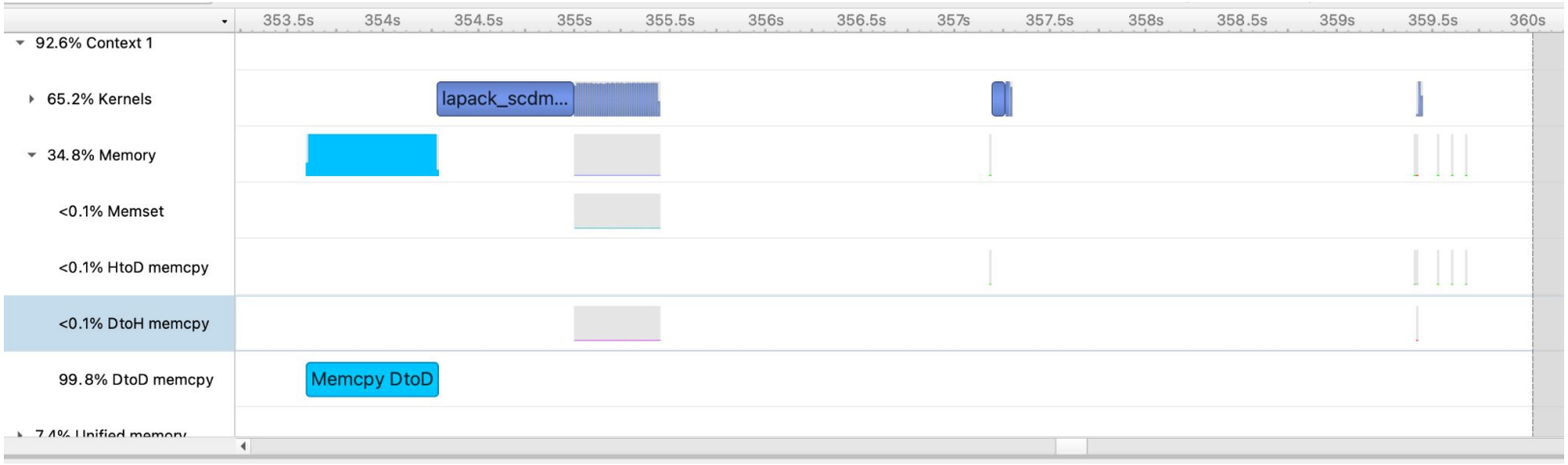
Hsin-Yu Ko et. Al. (under preparation)


Out-of-Sample: $(H_2O)_{512}$ @ 330 K
RMSE = 8.8×10^{-4} Ha/Bohr
DNN Forces (Ha/Bohr)
DFT Forces (Ha/Bohr)
0.08
0.04
0.00
−0.04
−0.08
−0.08
−0.04
0.00
0.04
0.08

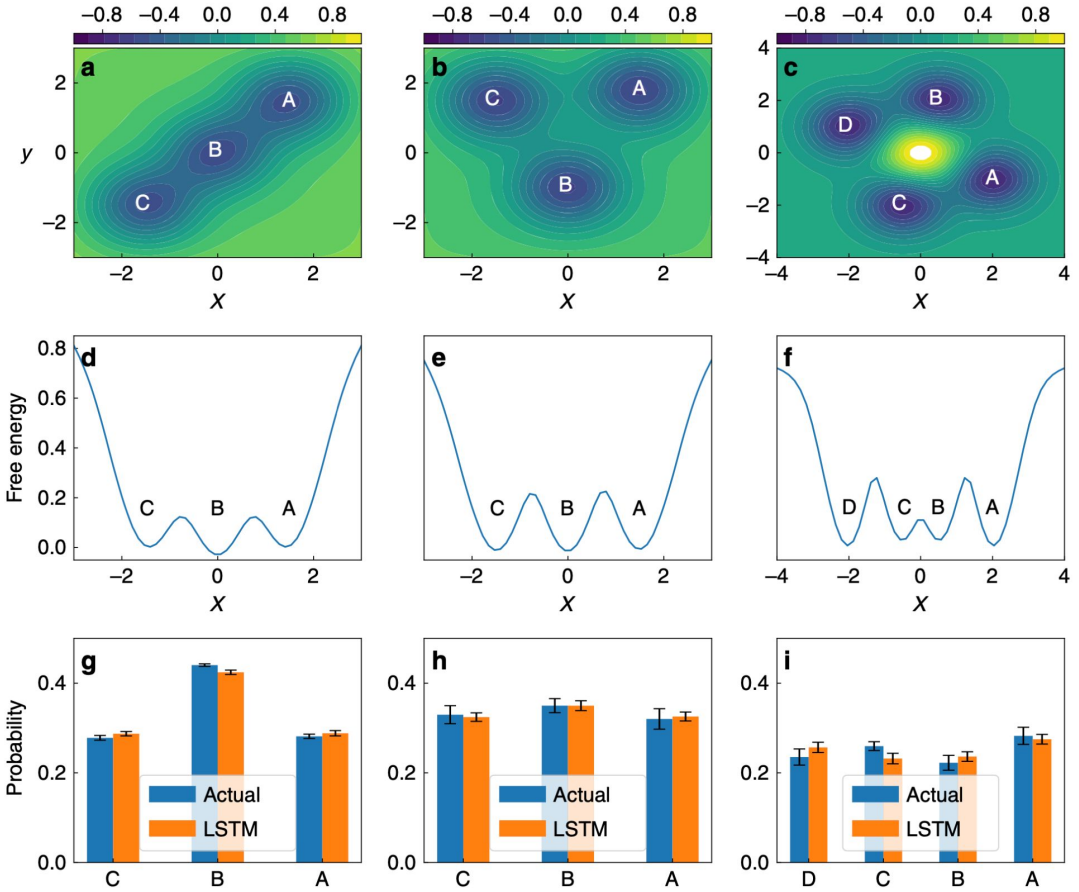
SCDM on GPU

- Custom QRCP with LAPACK/cuBLAS/cuLAPACK.
- Hybrid, highly scalable.

Nsight systems



ML in stochastic MD modelling



Sun-Ting Tsai, En-Jui Kuo and Pratyush Tiwari, Nat. Comm. (2020)

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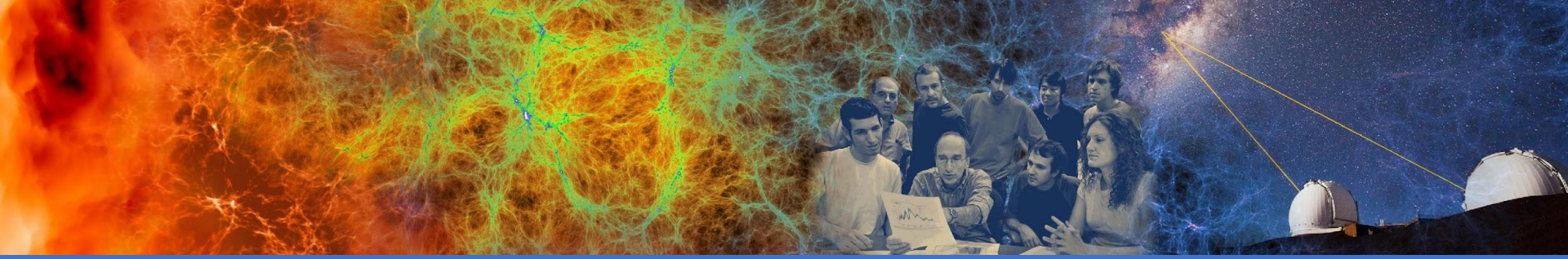
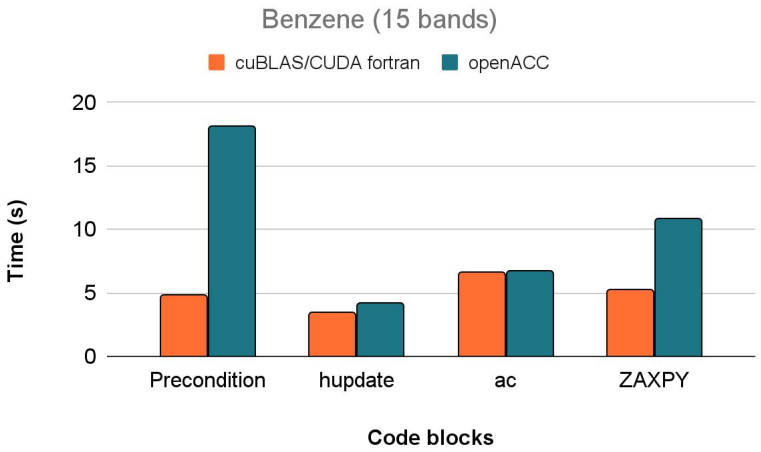
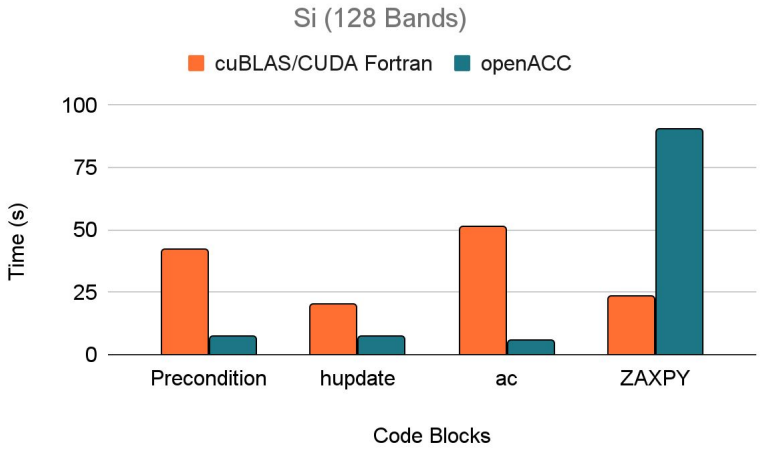


Porting to a device: Challenges, system-size, programming models

System-size dependence

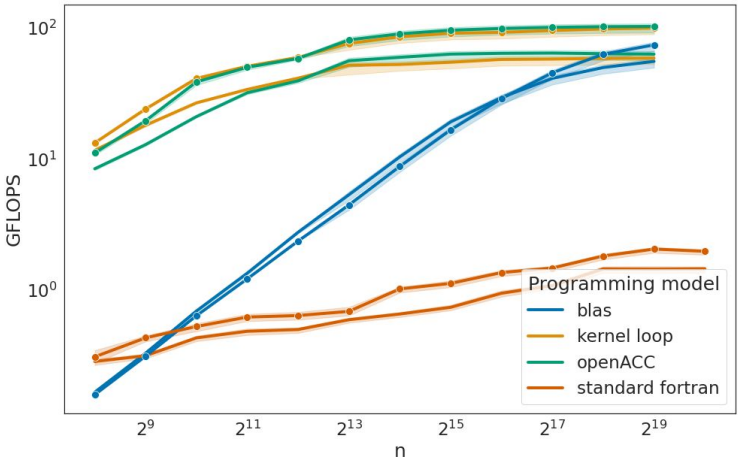




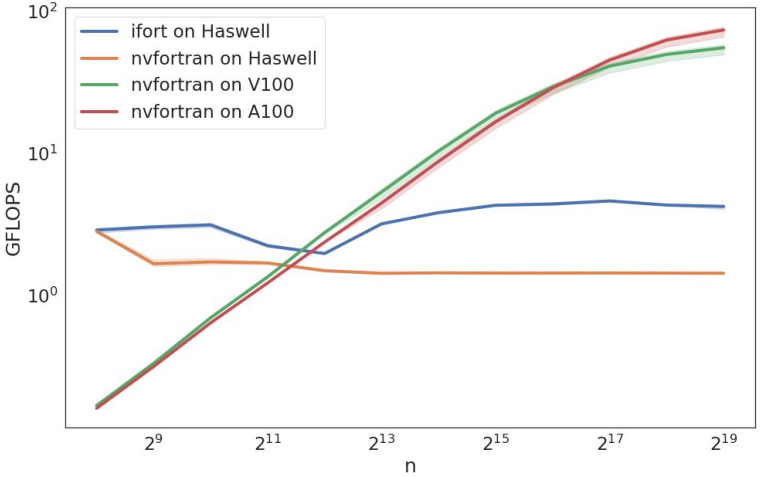
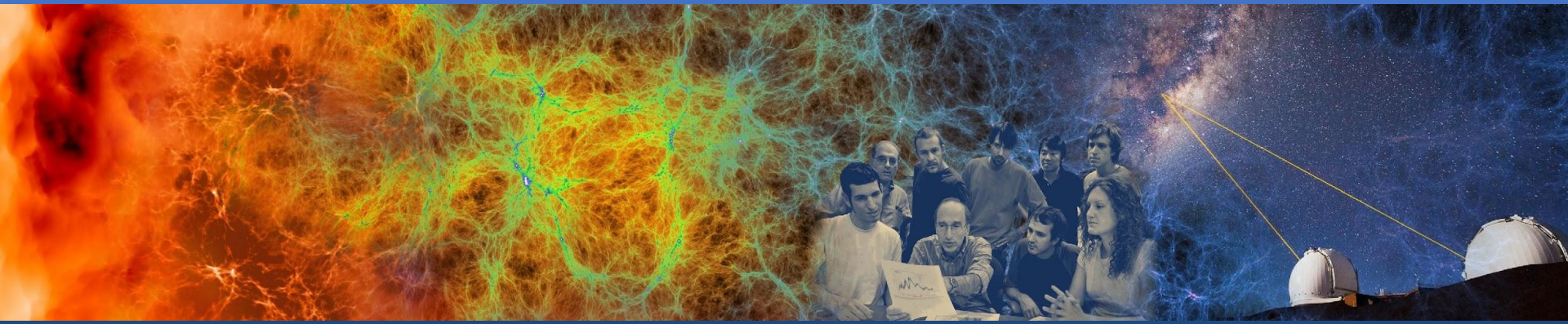
For constrained axpy, standard fortran is bad

$$Y = \alpha X + Y$$

OpenACC and cuf kernels are the best



AXPY BLAS saturates quickly on CPU



Thank You