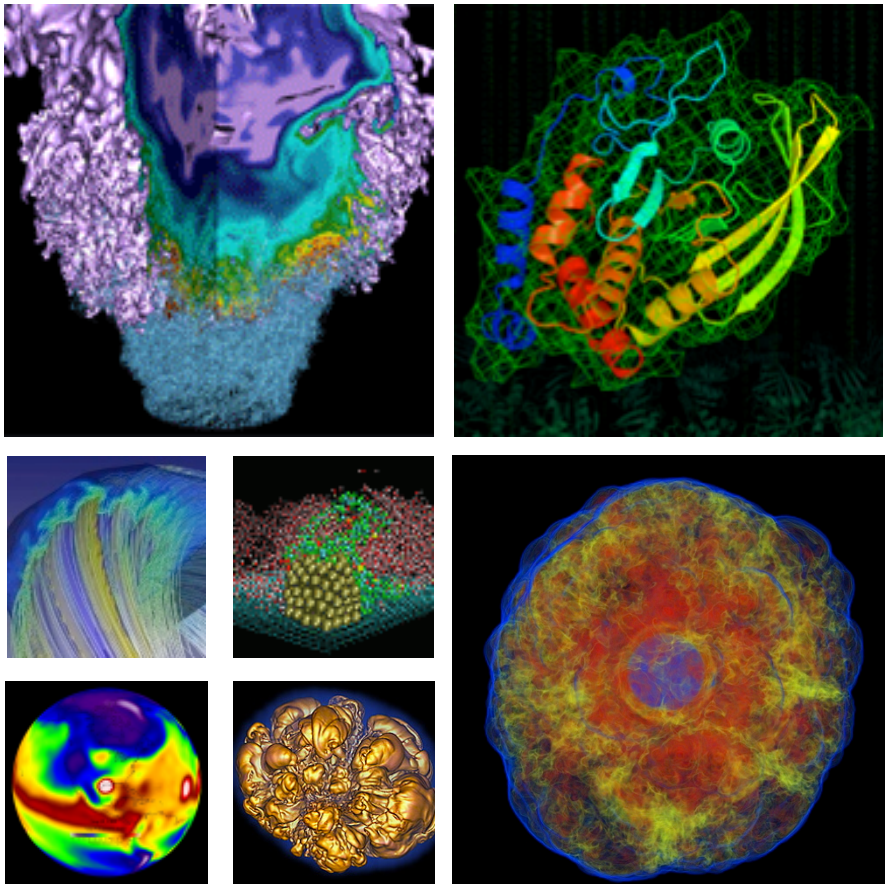
A Burst Buffer Use at NERSC



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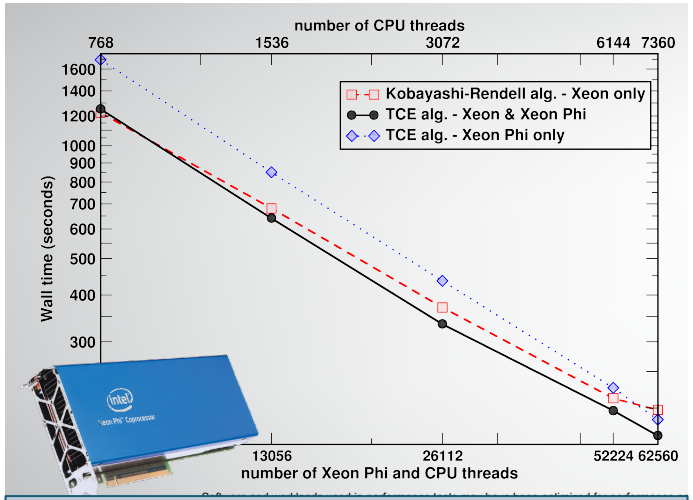
NWChem- Open Source High Performance Computational Chemistry Software

www.nwchem-sw.org

- NWChem is developed by a consortium of developers and maintained by the EMSL at PNNL.
- NWChem aims to provide its users with computational chemistry tools that are scalable both in their ability to treat large scientific computational chemistry problems efficiently, and in their use of available parallel computing resources from high-performance parallel supercomputers to conventional workstation clusters.
- Commonly used code at NERSC, and is one of the 20 NESAP codes under active development.



CCSD(T) on Intel Exon Phi: from Apra, Kowalski(PNNL), Klemm (Intel), "Efficient Implementation of Many Body Quantum Chemical Methods on the Xeon Phi Coprocessor", SC14.

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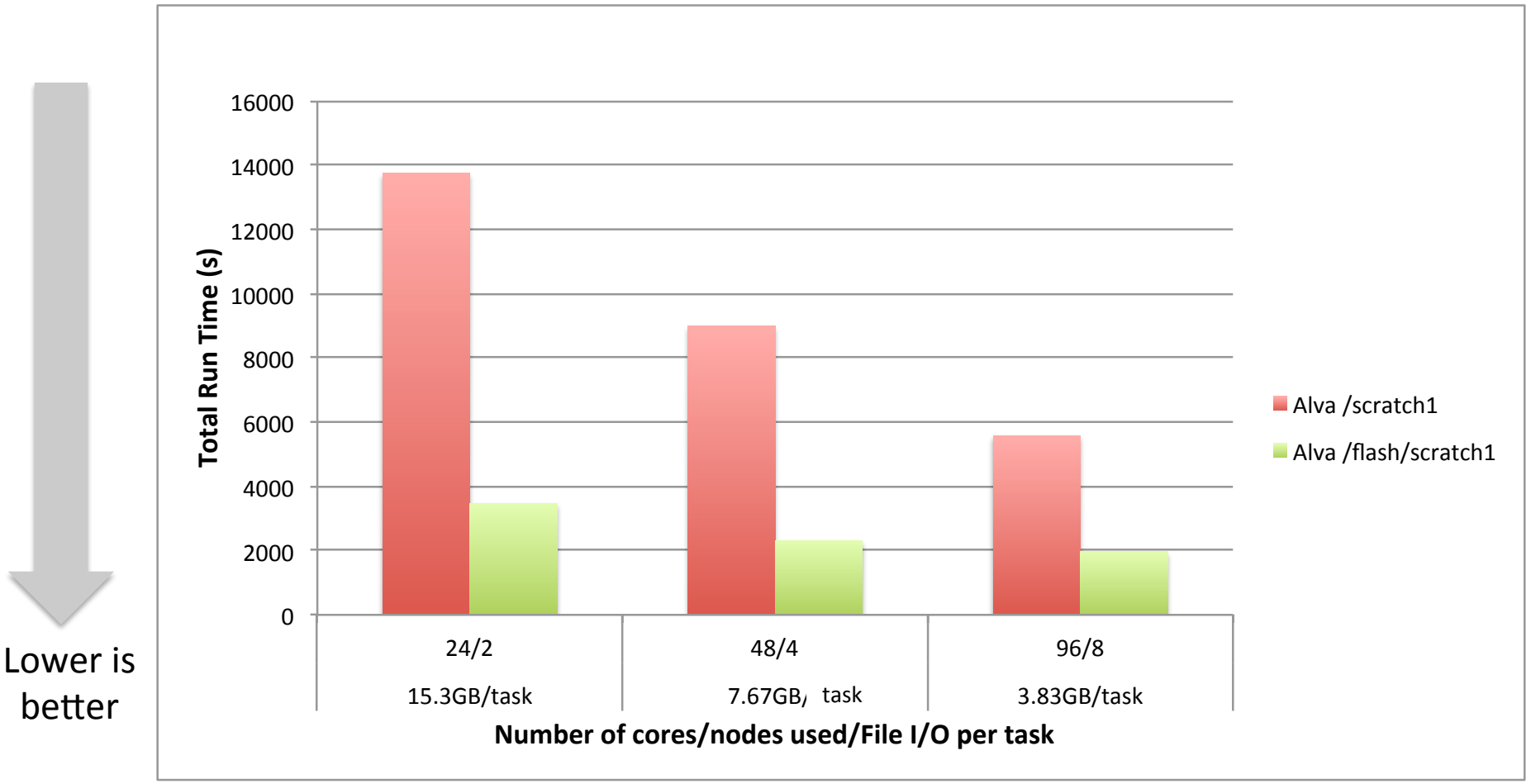
Figure provided by Eric Bylasca at PNNL

NWChem Out-of-Core Performance: Flash vs Disk on Burst Buffer testbed



- NWChem MP2 Semi-direct energy computation on 18 water cluster with aug-cc-pvdz basis set
- Geometry (18 water cluster) from A. Lagutschenkov, e.tal, *J. Chem. Phys.* **122**, 194310 (2005).

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