Computational Challenges in Cold QCD

Bálint Joó, Jefferson Lab

Computational Nuclear Physics Workshop

SURA

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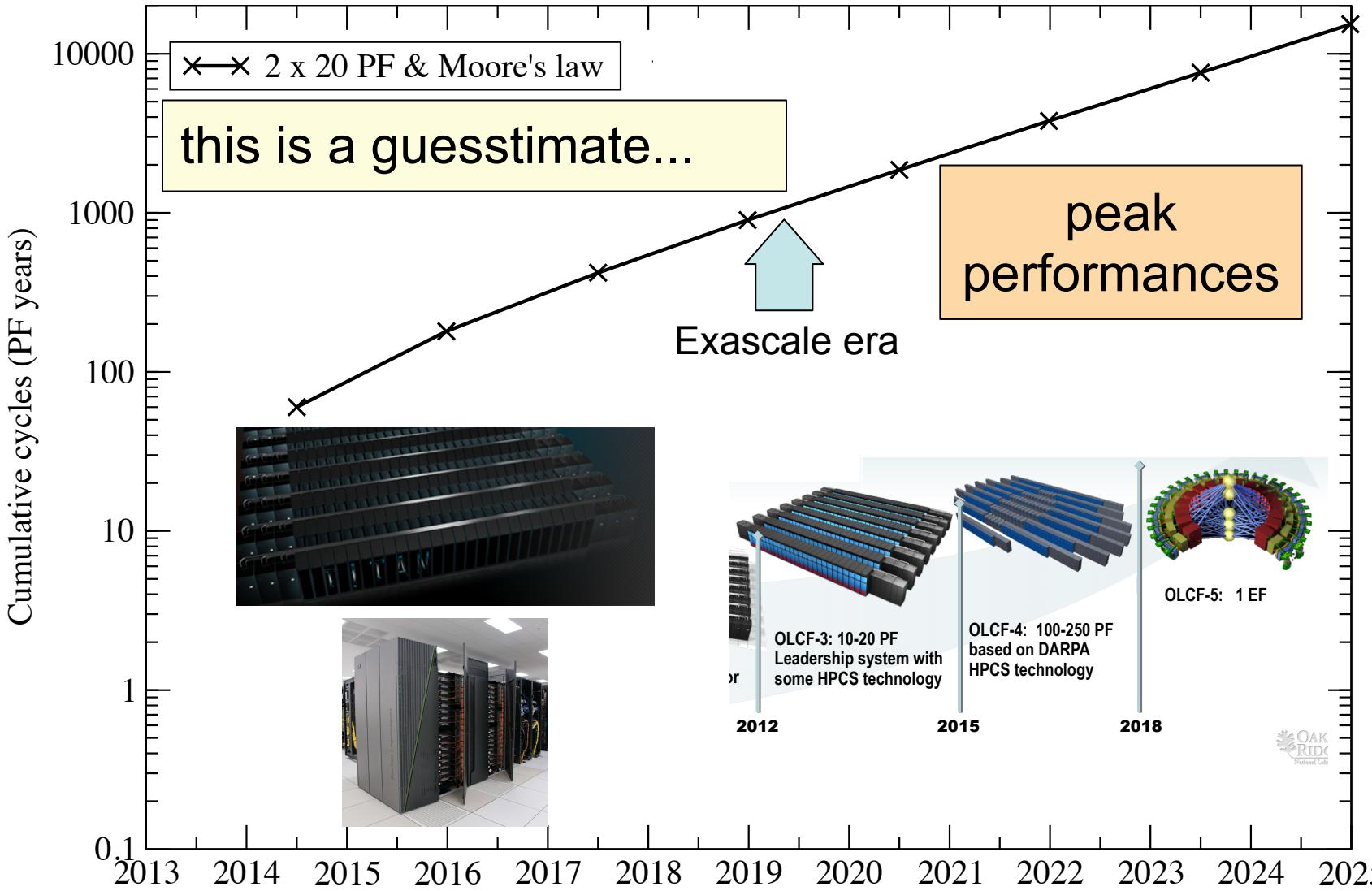
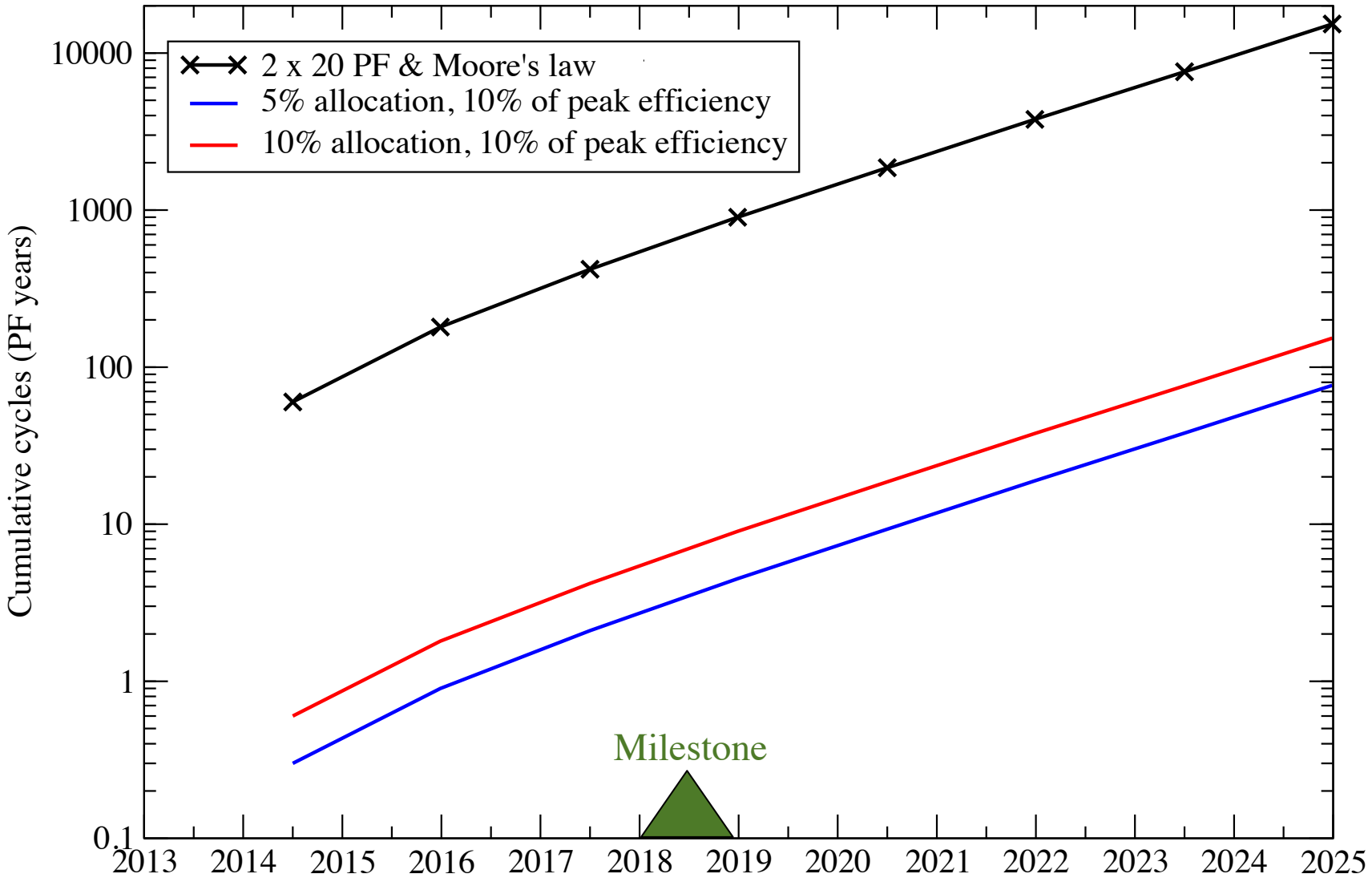
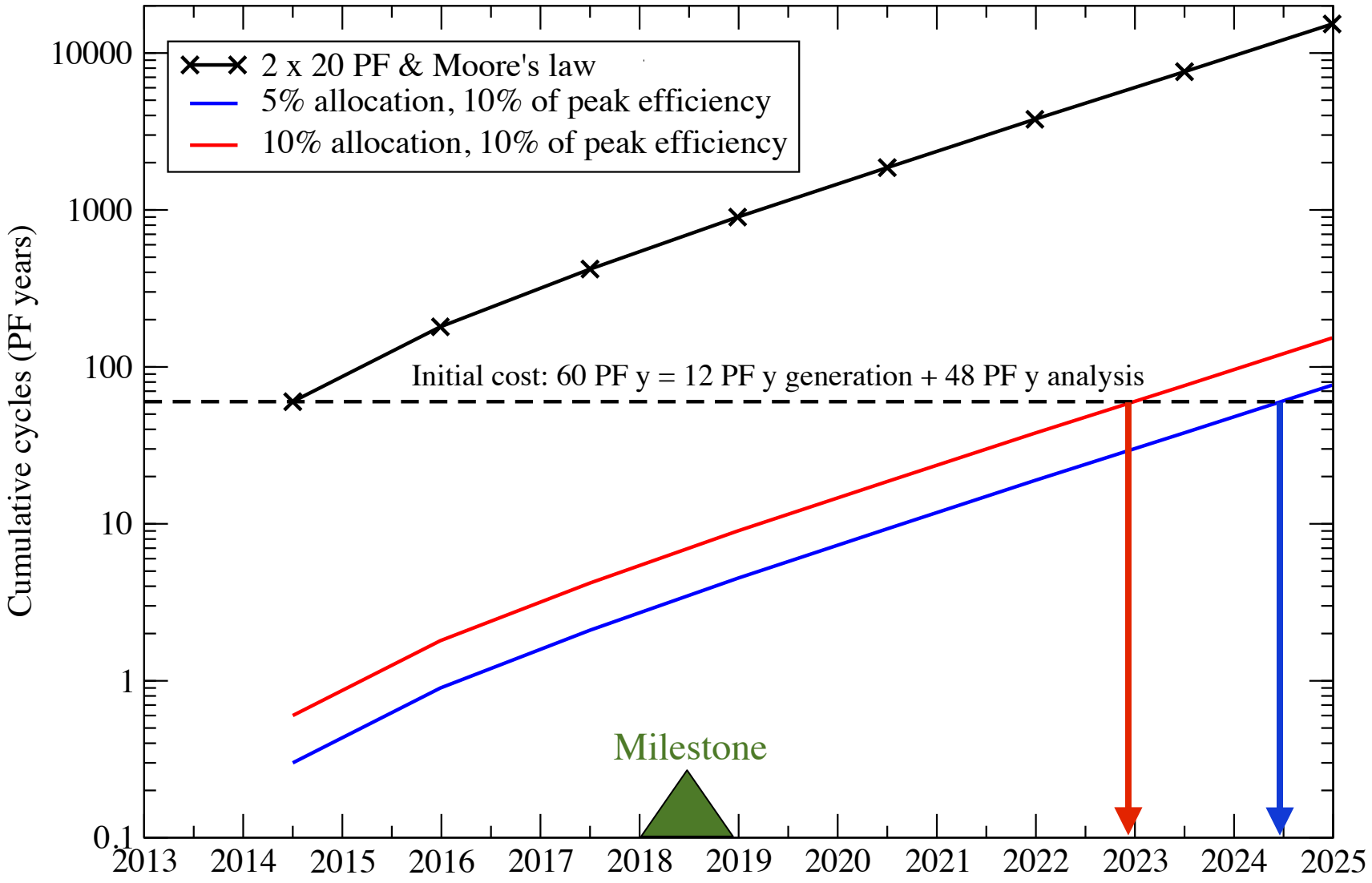
Cycles from Titan, Mira



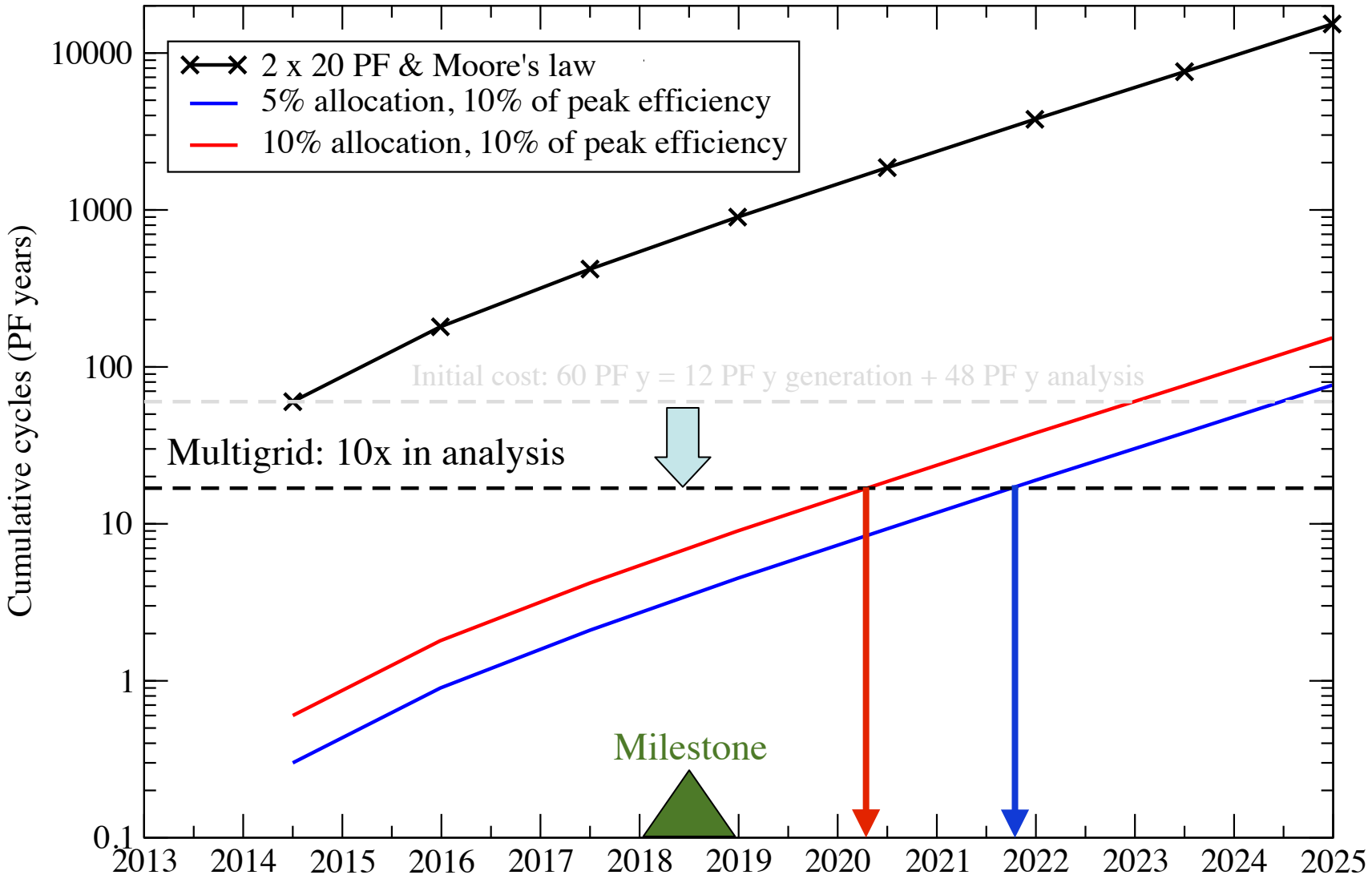
Cycles from Titan, Mira



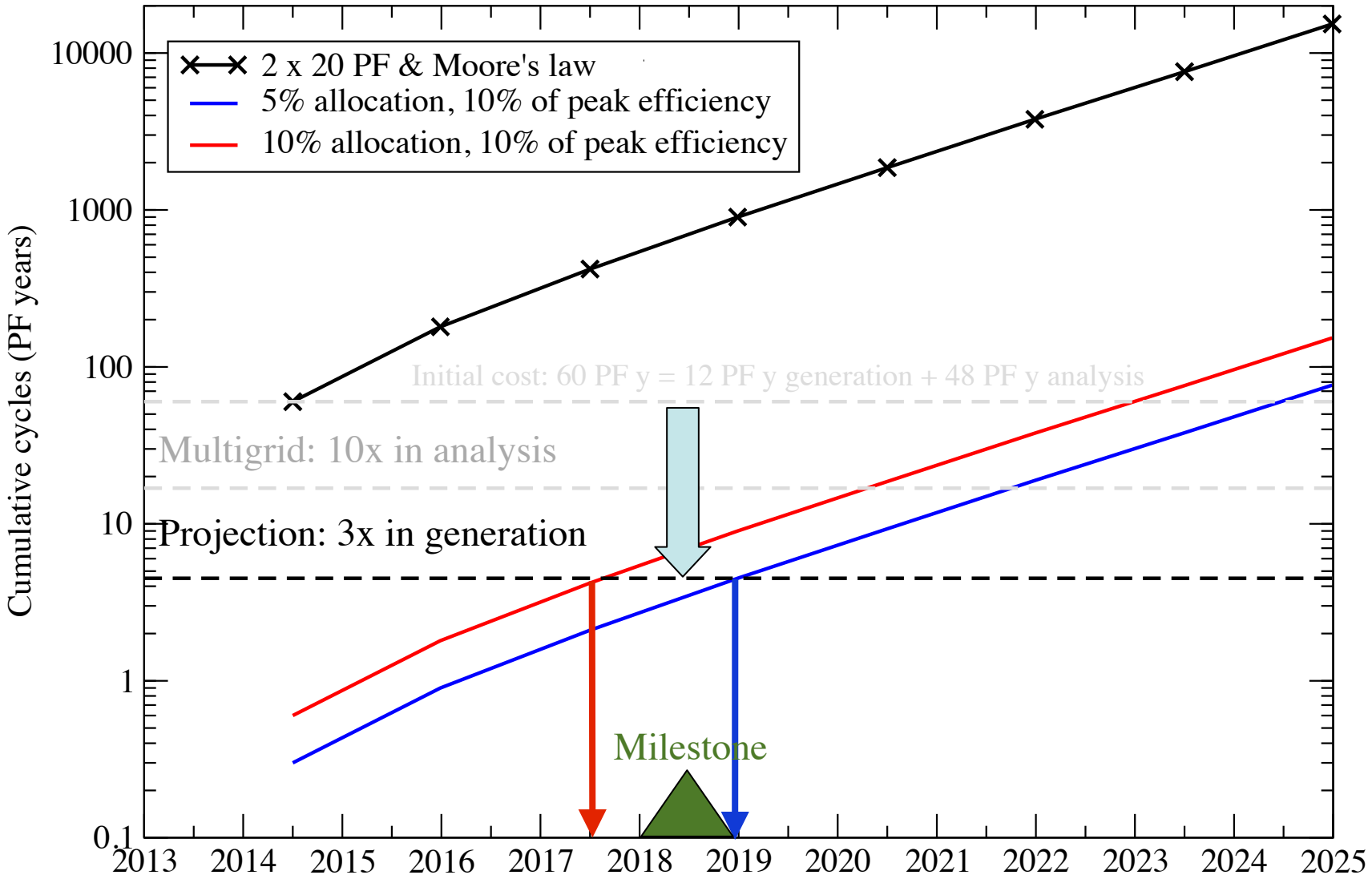
Sooner is better



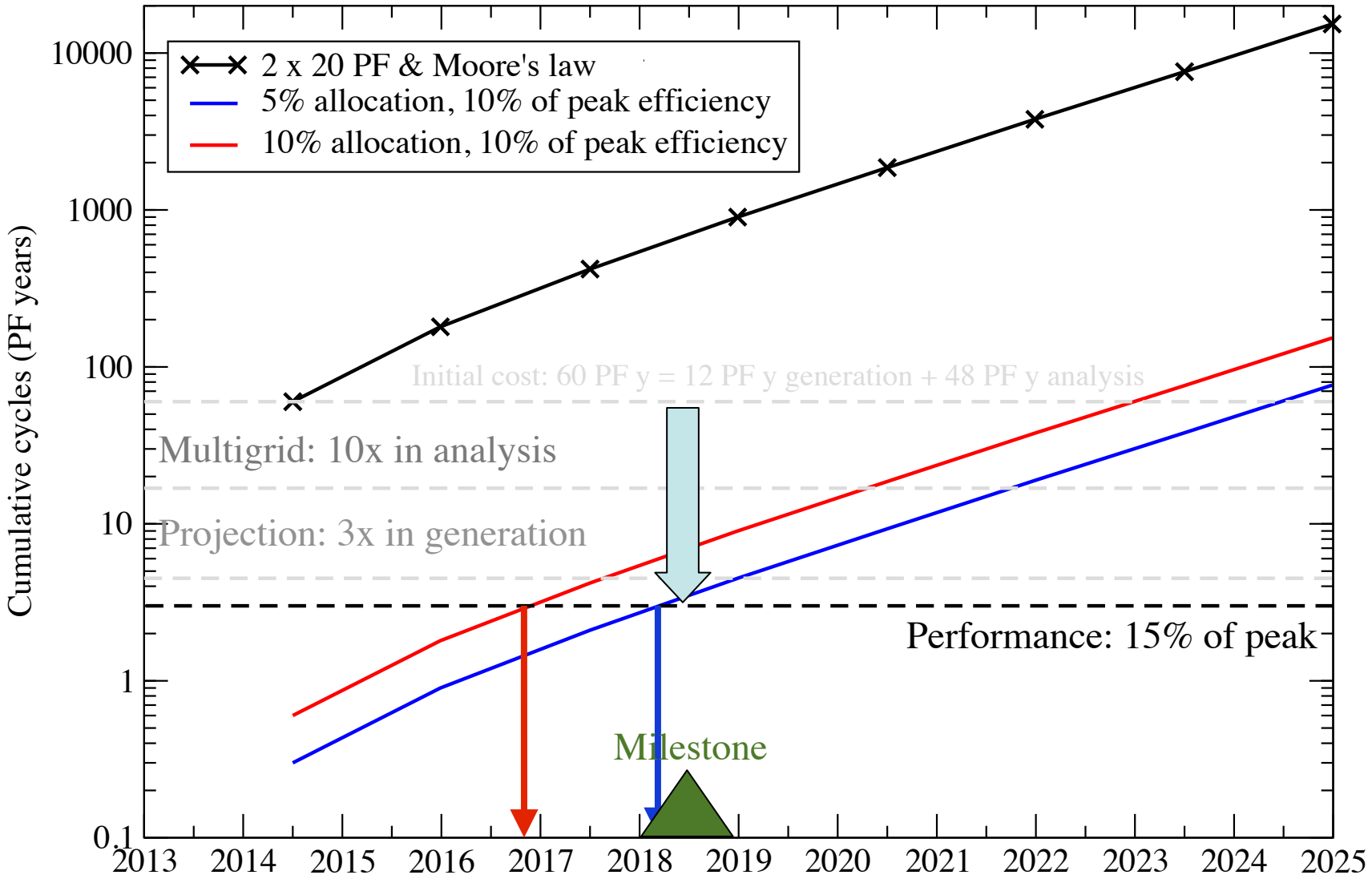
Improve Algorithms



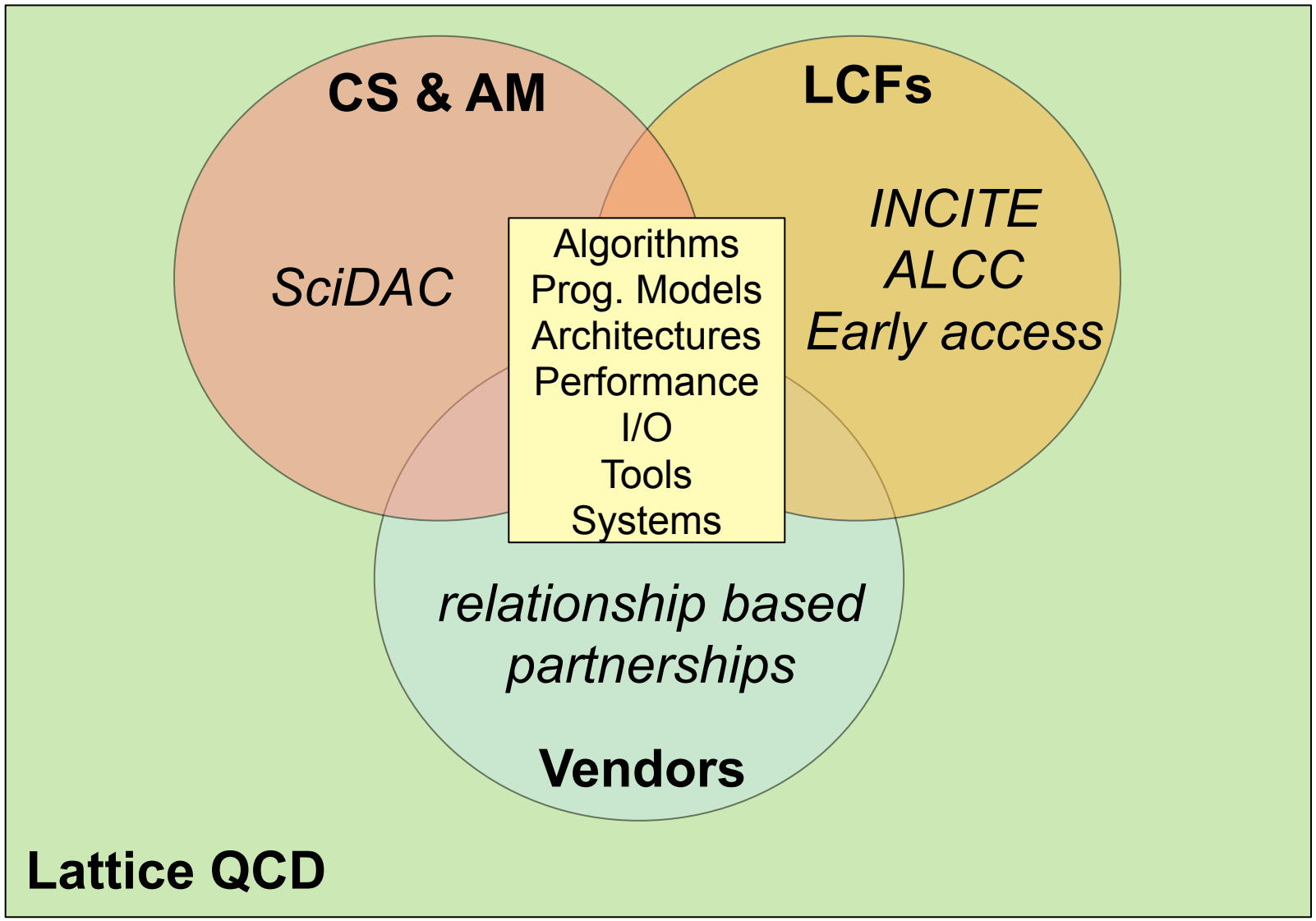
Improve Algorithms



Improve Performance



Required Partnerships



Algorithms and Architectures

- Improve algorithms & extract more performance
  - shift the cost down, to meet milestones
  - implement currently known techniques (e.g. MultiGrid)
- Partnerships with CS & AM: SciDAC
- Partnerships with Vendors
  - Co-design activity with IBM (BG/L & BG/Q)
  - Partnership with NVIDIA (GPUs)
  - Partnership with Intel (Xeon, MIC)
- Partnerships with Leadership Computing Facilities
  - Partnership with OLCF (TitanDev),
  - Partnership with ALCF (VEAS/VESTA, Mira)
  - Partnership with LLNL (Sequoia, Edge, uBGL)
  - Partnership with NSF Centers (Blue Waters, Stampede)
- Greatest impact is from software: need people

Exascale Era

- Concurrency:
  - In principle no problem:
    - O(10M) way now (lattice sites), O(100M-1000M) soon, V^4 growth
  - Difficulty is “portably efficient” mapping to hardware
    - Diverse architectures (Homogeneous Multicore, Heterogeneous Manycore)
    - Few vendor neutral performance portable programming models
  - Heterogeneity
    - Current LQCD GPU approaches ignore CPU
    - Need to develop truly heterogeneous approaches
- Resiliency
  - Some computations can be checked (e.g. Solves)
  - I/O & data management may become (already are?) issues
  - Will we need to change our methodology (?)

Staffing and Resource

- HPC is becoming an integral part of Nuclear Physics
  - lack of HPC training is already a disadvantage
- Need long term career structure for computational scientists
  - end “computing doesn’t lead to physics career” stereotype
- Useful to coordinate academic & technical positions
  - hire theoretical and computational staff together
    - e.g. faculty at local university, supporting computational staff at nearby center
- Industry and Leadership Facilities can play a strong role:
  - studentships, internships, training workshops
    - Develop skill-set, interest and experience early on
  - liaisons
    - Maintain awareness of QCD
    - Provide guidance for architectures, systems, and policies for QCD needs

Summary & Conclusions

- In order to meet the Scientific Milestones QCD will need:
  - increased levels of HPC (cycles)
  - capability on both homogeneous & heterogeneous H/W
  - investment in algorithmic and programming model research
  - strong links between domain, AM & CS communities
  - strong partnerships with LCFs and Vendors to anticipate and influence architectures and systems
- Meeting these needs requires an increase in staffing
  - both short and long term
  - to cope with architectural diversity
  - to develop algorithms and methodology towards exascale
  - to enable scientists to ‘choose computational’ as a career