Towards Building Blocks for Autonomous Science Infrastructure

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Science vs Commercial Infrastructure

- Different types of “scale”, optimization, customization
  - Science: Scaling single applications/workflows
  - Commercial: Scaling the number of users
- Autonomous Capabilities (Objectives)
  - System Performance based vs “abstract” science based
  - System-level vs user-level autonomous functionality
- Software systems to support autonomous capabilities
  - Self-* systems: Used in data centers; few application / algorithm
  - Diverse “design points”; unlikely “one size fits all”; last mile distinction

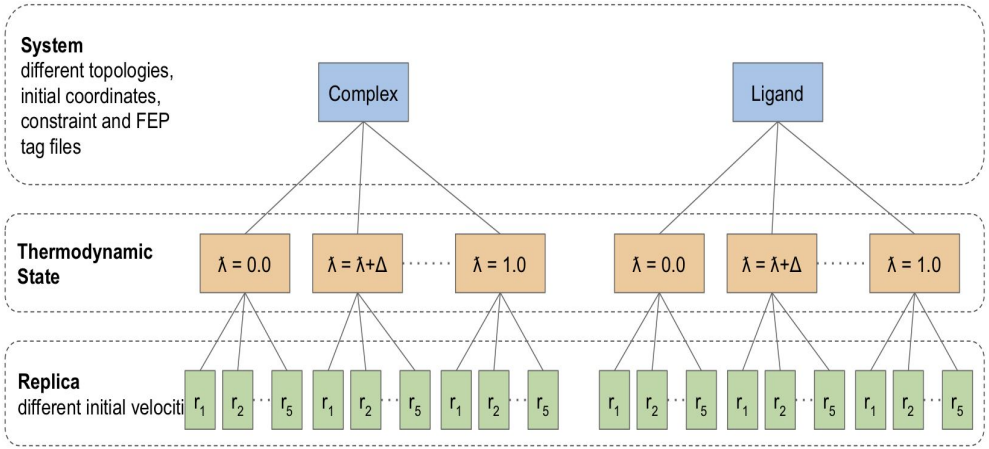
Three Examples

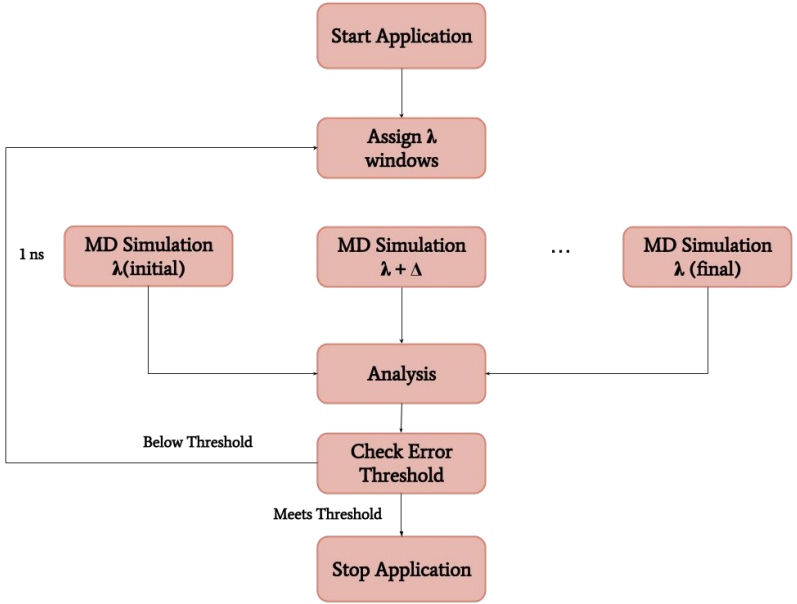
- Autonomic Workload Management Systems: Distributed
  - Automated mapping of heterogeneous tasks to resources
  - Yields improvement in system response time and system utilization.
- Autonomic Workload Management Systems: HPC
  - “Performance Portability” is ultimate goal. “Shapeshifting resources” to provide weaker guarantees on performance is acceptable!
- Support for Optimal Execution Strategies at Scale
  - Not how much you use, but what you do with it
    - Bigger is not automatically better. Bigger but also better!
  - Middleware and workflow systems for Adaptive Execution @ Exascale

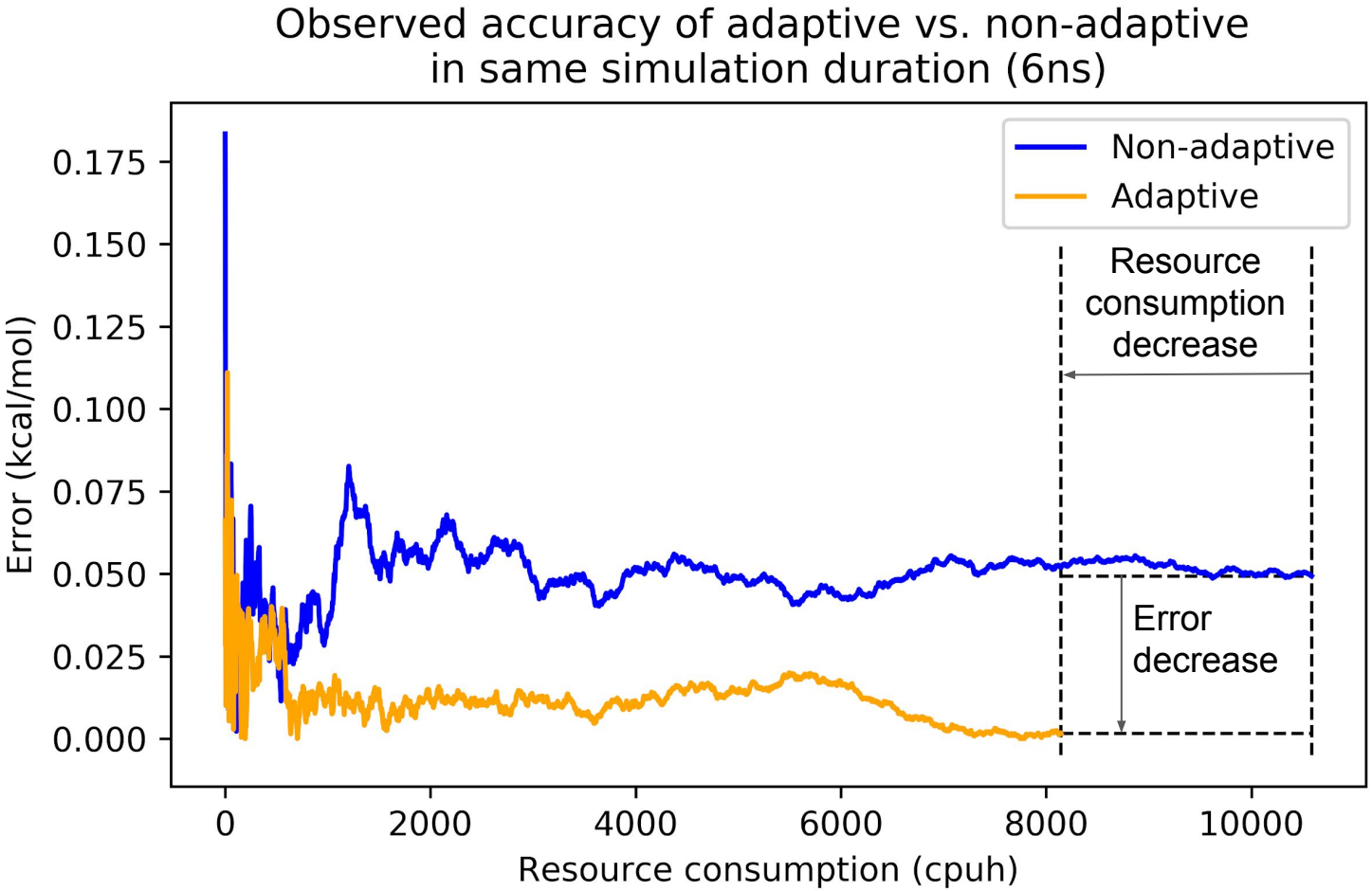
TIES Protocol for Binding Free Affinity

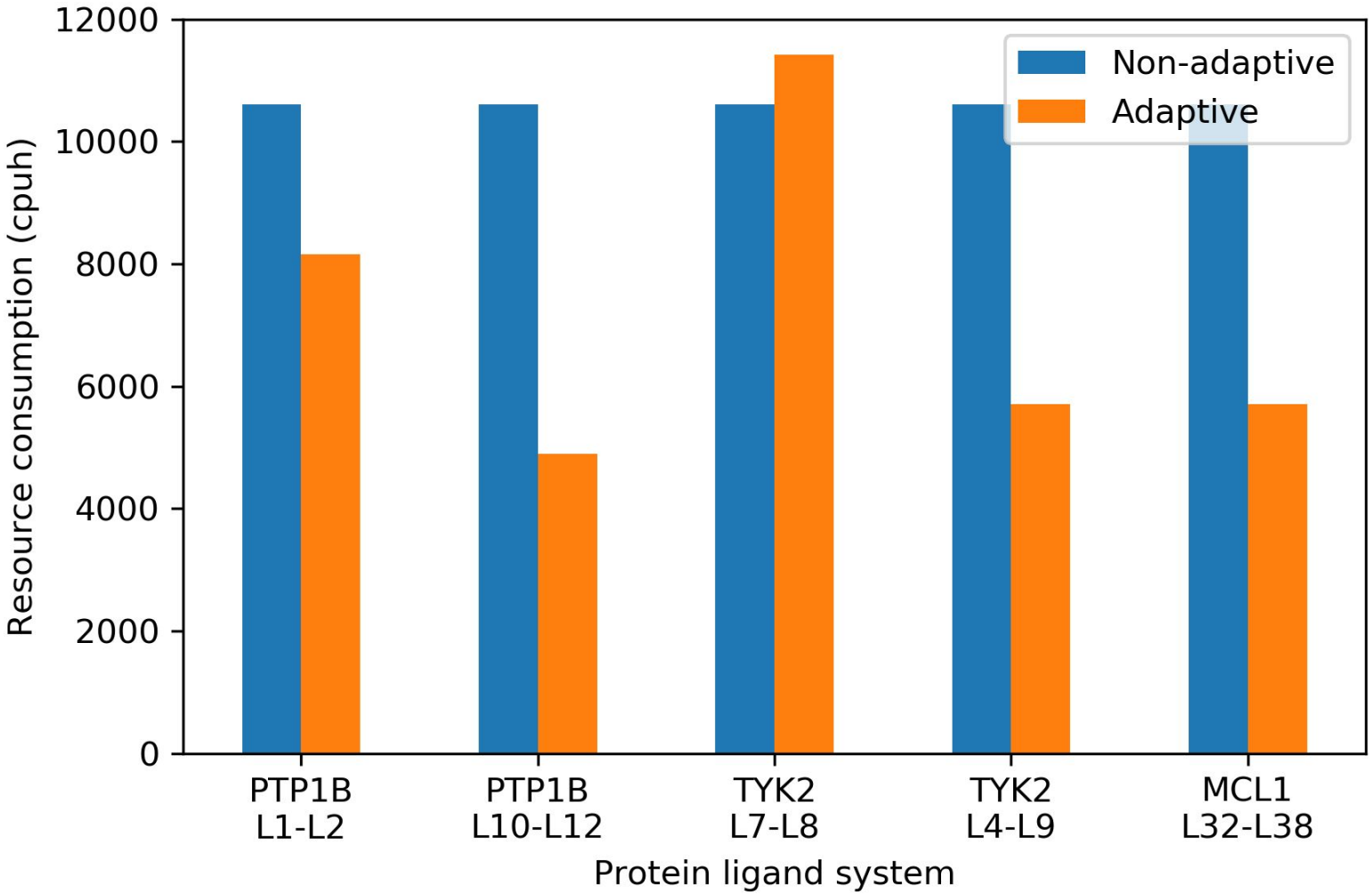
TIES (alchemical **protocol**) employs enhanced sampling at each lambda window to yield relative binding affinities.

Adaptive quadrature algorithm adds additional simulations or modified lambda values to reduce error on binding free affinity.






Observed accuracy of adaptive vs. non-adaptive
in same simulation duration (6ns)
Non-adaptive
Adaptive
Resource
consumption
decrease
Error
decrease
Error (kcal/mol)
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
0
2000
4000
6000
8000
10000
Resource consumption (cpuh)


12000
10000
8000
6000
4000
2000
0
Resource consumption (cpuh)
Non-adaptive
Adaptive
PTP1B
L1-L2
PTP1B
L10-L12
TYK2
L7-L8
TYK2
L4-L9
MCL1
L32-L38
Protein ligand system