***N* Tropy**: A Framework for Parallel Data Analysis

Harnessing the Power of Parallel Grid Resources for Astronomical Data Analysis

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TERAGRID

Mining the Universe can be Computationally Expensive

- Astronomy now generates ~ 1TB data per night
- With VOs, one can pool data from multiple catalogs.
- Computational requirements are becoming much more extreme relative to current state of the art.
- There will be many problems that would be impossible without parallel machines.
- Example: N-Point correlation functions for the SDSS
  - 2-pt: CPU hours
  - 3-pt: CPU weeks
  - 4-pt: 100 CPU years!
- There will be many more problems for which throughput can be substantially enhanced by parallel machines.

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Types of Parallelism

- Data Parallel (or “Embarrassingly Parallel”):
  - Example:
    - 100,000 QSO spectra
    - Each spectrum takes ~1 hour to reduce
    - Each spectrum is computationally independent from the others
  - If you have root access to a Grid resource:
    - Solution for “traditional” enviroment: Condor
    - VOs will provide a integrated workflow solution (e.g. Pegasus)
  - Running on shared resources like the TeraGrid is more difficult
    - TeraGrid has no metascheduler
    - TeraGrid batch systems cannot handle 100,000 independent work units
    - Solution: GridShell (talk to me if you are interested!)

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Types of Parallelism

- Tightly Coupled Parallelism (What this talk is about):
  - Data and computational domains overlap
  - Examples:
    - N-Point correlation functions
    - New object classification
    - Density estimation
    - Intersections in parameter space
  - Solution(?):
    - *N* Tropy

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The Challenge of Parallel Data Analysis

- Parallel programs are hard to write!
  - Steep learning curve to learn parallel programming
  - Lengthy development time
- Parallel world is dominated by simulations:
  - Code is often reused for many years by many people
  - Therefore, you can afford to spend lots of time writing the code.
- Data Analysis does not work this way:
  - Rapidly changing scientific inqueries
  - Less code reuse
- Data Analysis requires rapid software development!
- Even the simulation community rarely does data analysis in parallel.

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The Goal

- GOAL: Minimize development time for parallel applications.
- GOAL: Allow scientists who don't have the time to learn how to write parallel programs to still implement their algorithms in parallel.
- GOAL: Provide seamless scalability from single processor machines to TeraGrid platforms
- GOAL: Do not restrict inquiry space.

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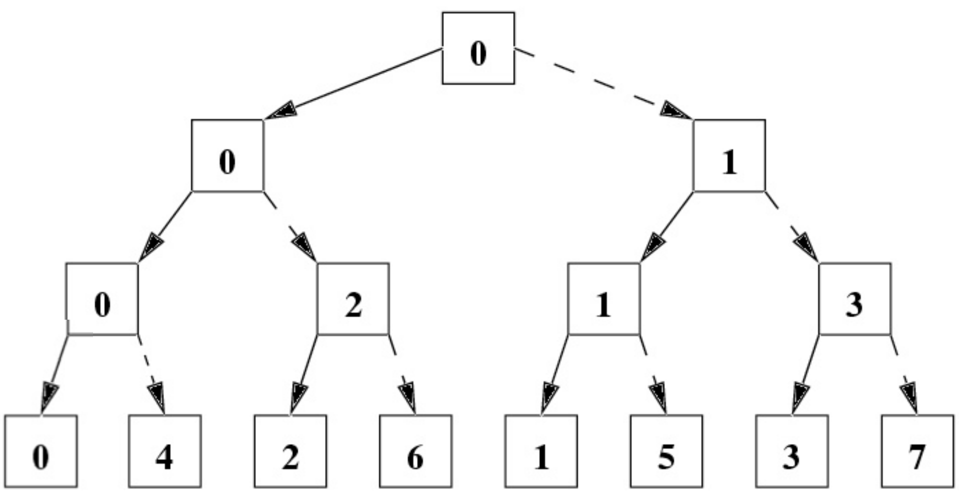
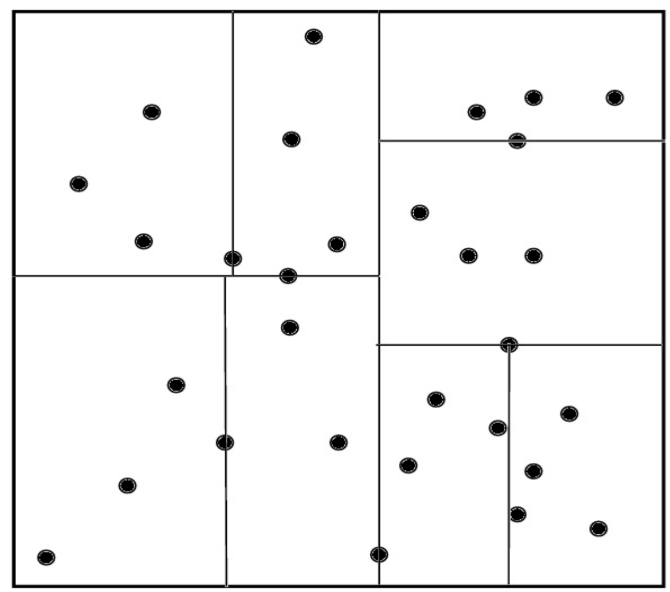
Methodology

- Limited Data Structures:
  - Most (all?) efficient data analysis methods use grids or trees.
- Limited Methods:
  - Analysis methods perform a limited number of operations on these data structures.





Methodology

- **Examples**:
  - Fast Fourier Transform
    - Abstraction: Grid
    - Method: Global Reduction
  - N-Body Gravity Calculation
    - Abstraction: Tree
    - Method: Global Top-Down TreeWalk
  - 2-Point Correlation Function Calculation
    - Abstraction: Tree
    - Method: Global Top-Down TreeWalk

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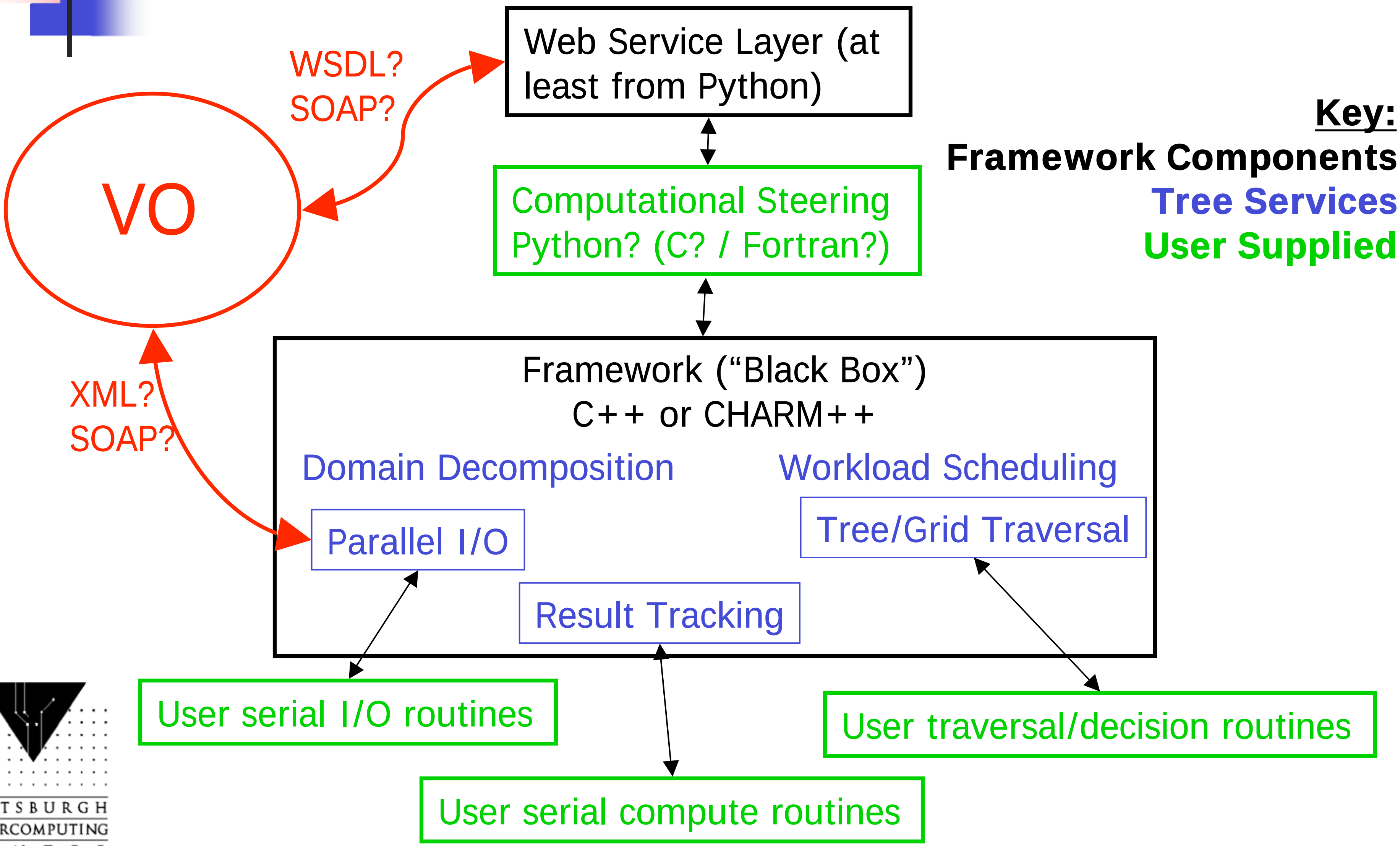
Vision: A Parallel Framework



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Proof of Concept: PHASE 1
(complete)

- Convert parallel N-Body code "PKDGRAV*" to 3-point correlation function calculator by modifying existing code as little as possible.
  - *PKDGRAV developed by Tom Quinn, Joachim Stadel, and others at the University of Washington
- PKDGRAV (aka GASOLINE) benefits:
  - Highly portable
    - MPI, POSIX Threads, SHMEM, Quadrics, & more
  - Highly scalable
    - 92% linear speedup on 512 processors
- Development time:
  - Writing PKDGRAV: ~10 FTE years (could be rewritten in ~2)
  - PKDGRAV -> 2-Point: 2 FTE weeks
  - 2-Point -> 3-Point: >3 FTE months

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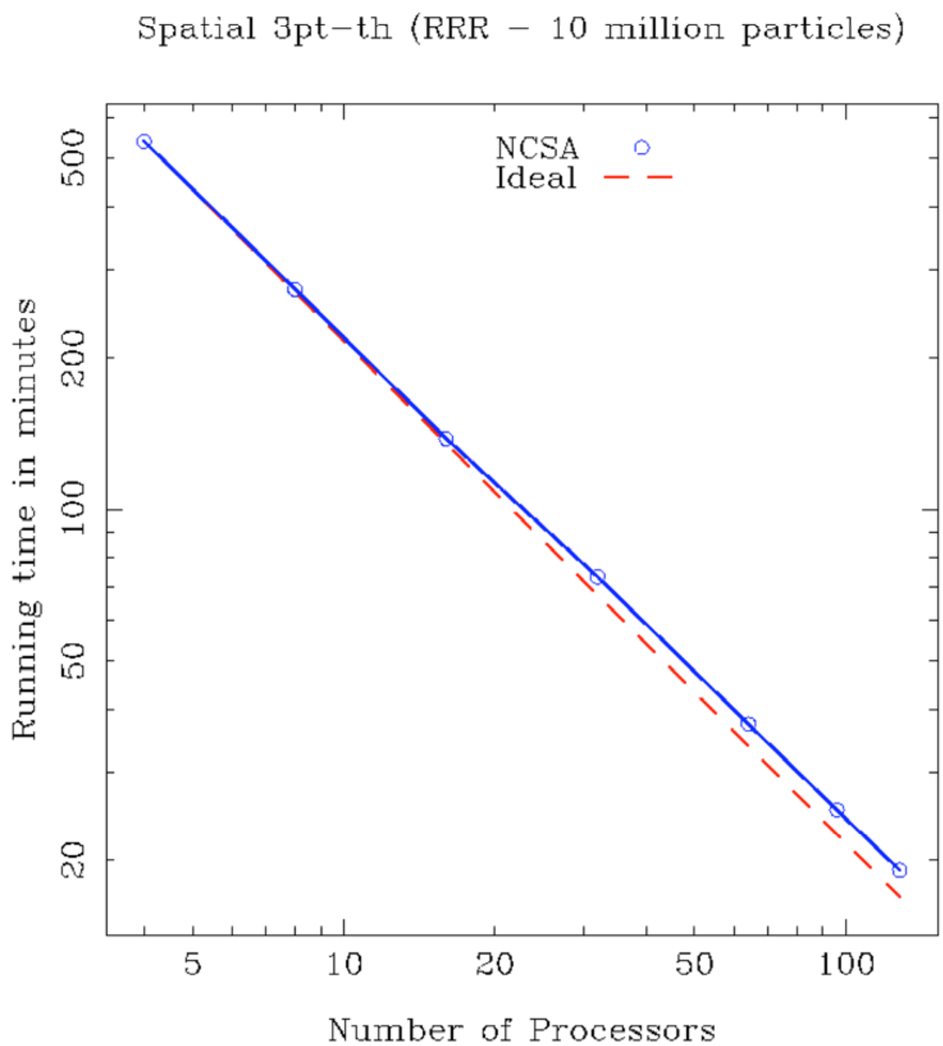
PHASE 1 Performance

10 million particles
Spatial 3-Point
3->4 Mpc

(SDSS DR1 takes less than 1 minute with perfect load balancing)



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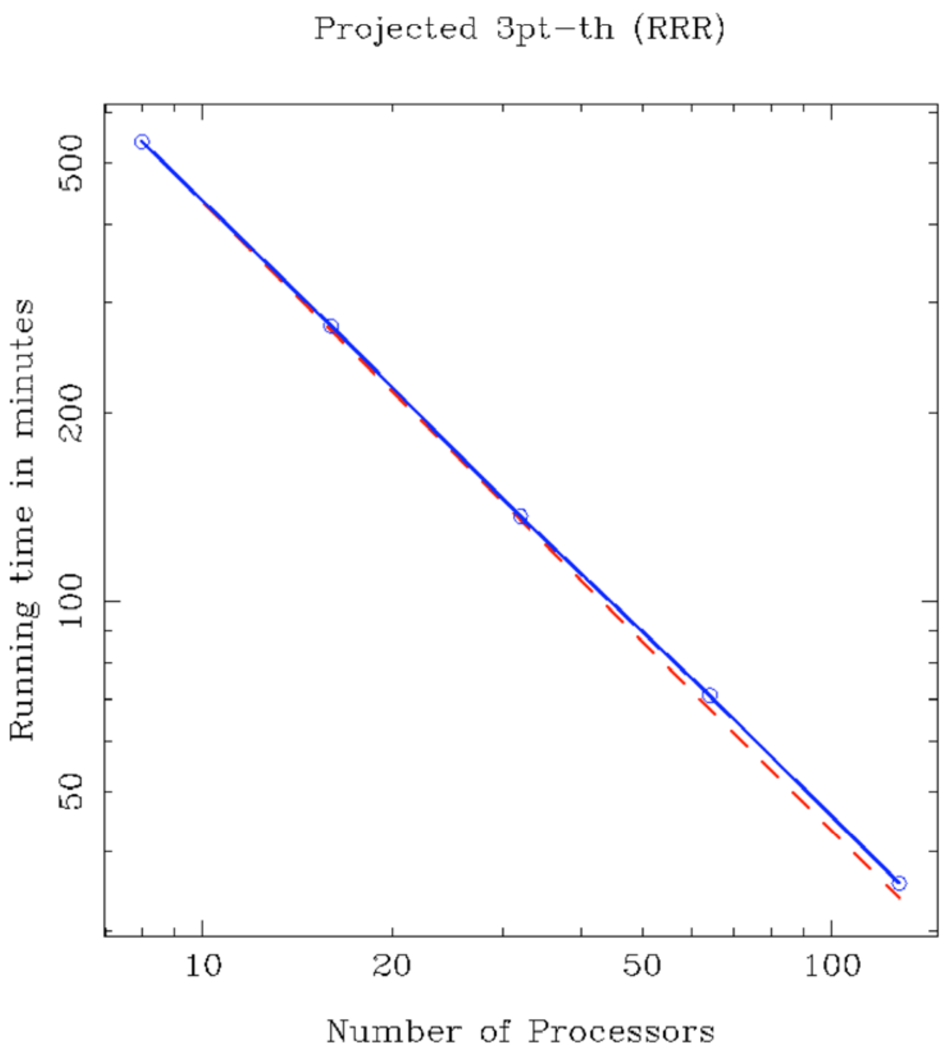
PHASE 1 Performance

10 million particles
Projected 3-Point
0->3 Mpc



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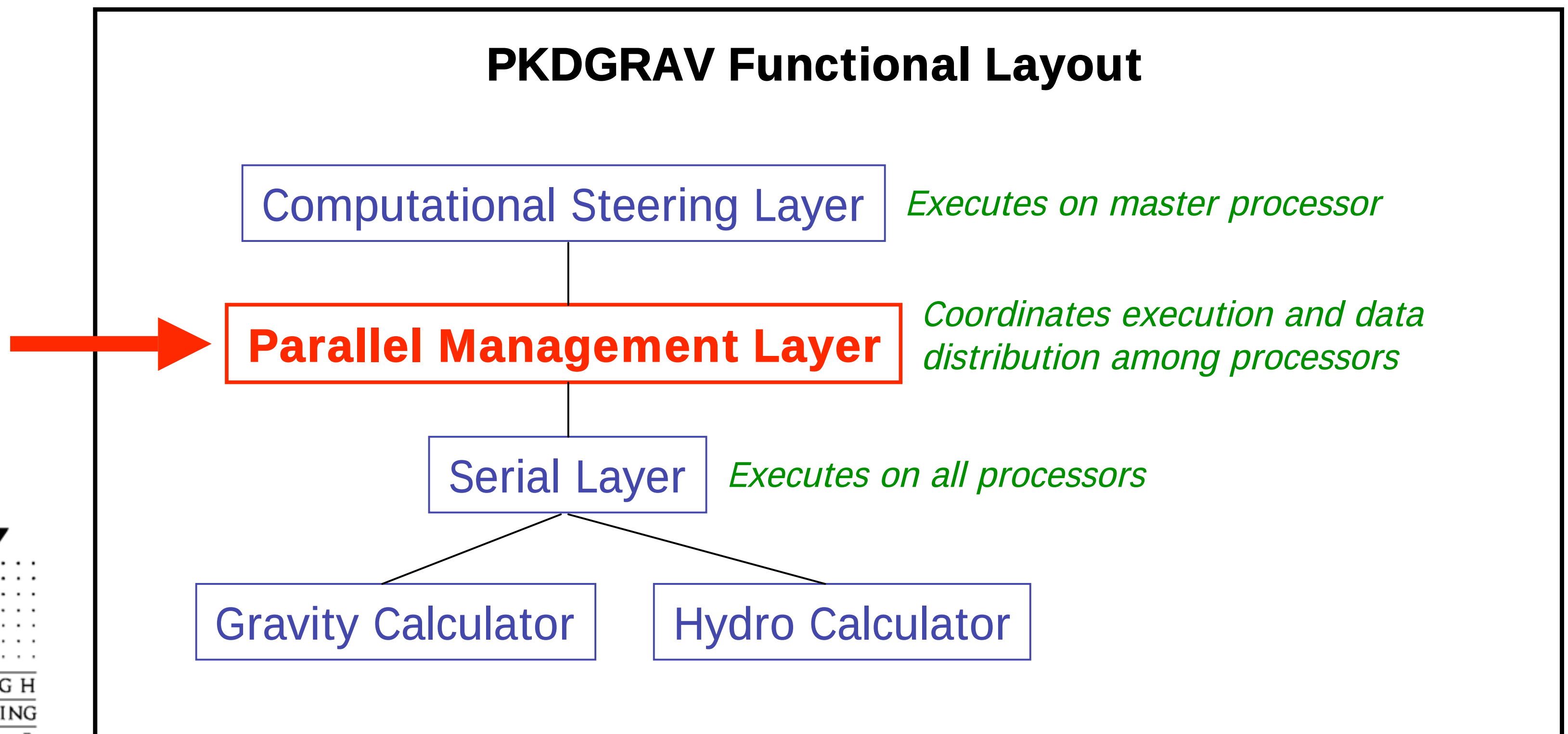
Proof of Concept: PHASE 2
N Tropy

(Currently in progress)

- Use only Parallel Management Layer of PKDGRAV.
- Rewrite everything else from scratch



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Proof of Concept: PHASE 2
N Tropy
(Currently in progress)

- Use only Parallel Managment Layer of PKDGRAV.
- Rewrite everything else from scratch
- PKDGRAV benefits to keep:
  - Flexible client-server scheduling architecture
    - Threads respond to service requests issued by master.
    - To do a new task, simply add a new service.
  - Portability
    - Interprocessor communication occurs by high-level requests to “Machine-Dependent Layer” (MDL) which is rewritten to take advantage of each parallel architecture.
  - Advanced interprocessor data caching
    - < 1 in 100,000 off-PE requests actually result in communication.

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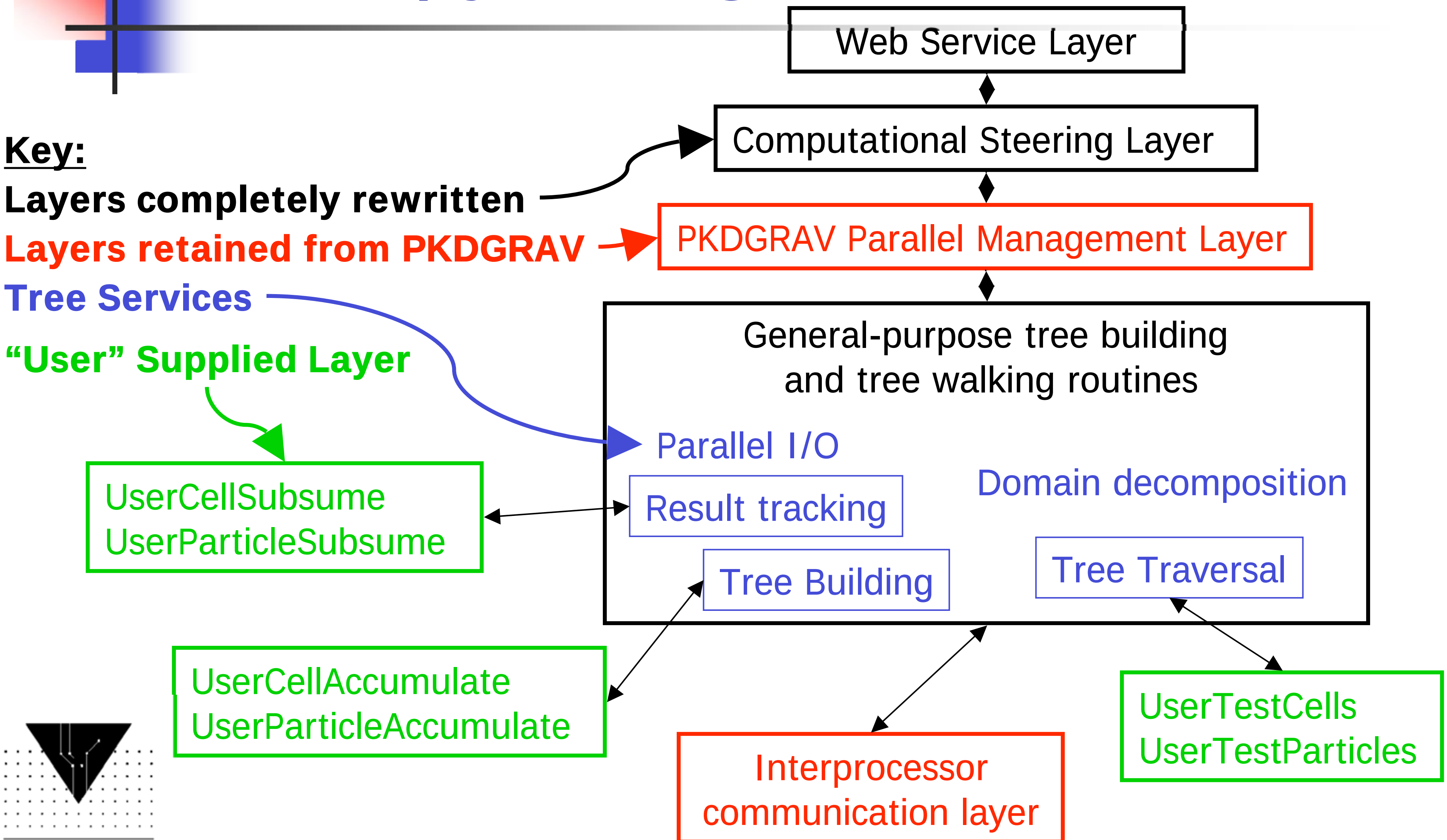
N Tropy Design

2-Point and 3-Point algorithm are now complete!



N Tropy "Meaningful" Benchmarks

- The purpose of this framework is to minimize development time!
- Rewriting user and scheduling layer to do an N-body gravity calculation:

N Tropy "Meaningful" Benchmarks

- The purpose of this framework is to minimize development time!
- Rewriting user and scheduling layer to do an N-body gravity calculation:

3 Hours

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N Tropy New Features
(coming soon)

- Dynamic load balancing
  - Workload and processor domain boundaries can be dynamically reallocated as computation progresses.
- Data pre-fetching
  - Predict request off-PE data that will be needed for upcoming tree nodes.
  - Work with CMU Auton-lab to investigate active learning algorithms to prefetch off-PE data.

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N Tropy New Features
(coming soon)

- Computing across grid nodes
  - Much more difficult than between nodes on a tightly-coupled parallel machine:
    - Network latencies between grid resources 1000 times higher than nodes on a single parallel machine.
  - Nodes on a far grid resources must be treated differently than the processor next door:
    - Data mirroring or aggressive prefetching.
    - Sophisticated workload management, synchronization

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Conclusions

- Most data analysis in astronomy is done using trees as the fundamental data structure.
- Most operations on these tree structures are functionally identical.
- Based on our studies so far, it appears feasible to construct a general purpose parallel framework that users can rapidly customize to their needs.

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