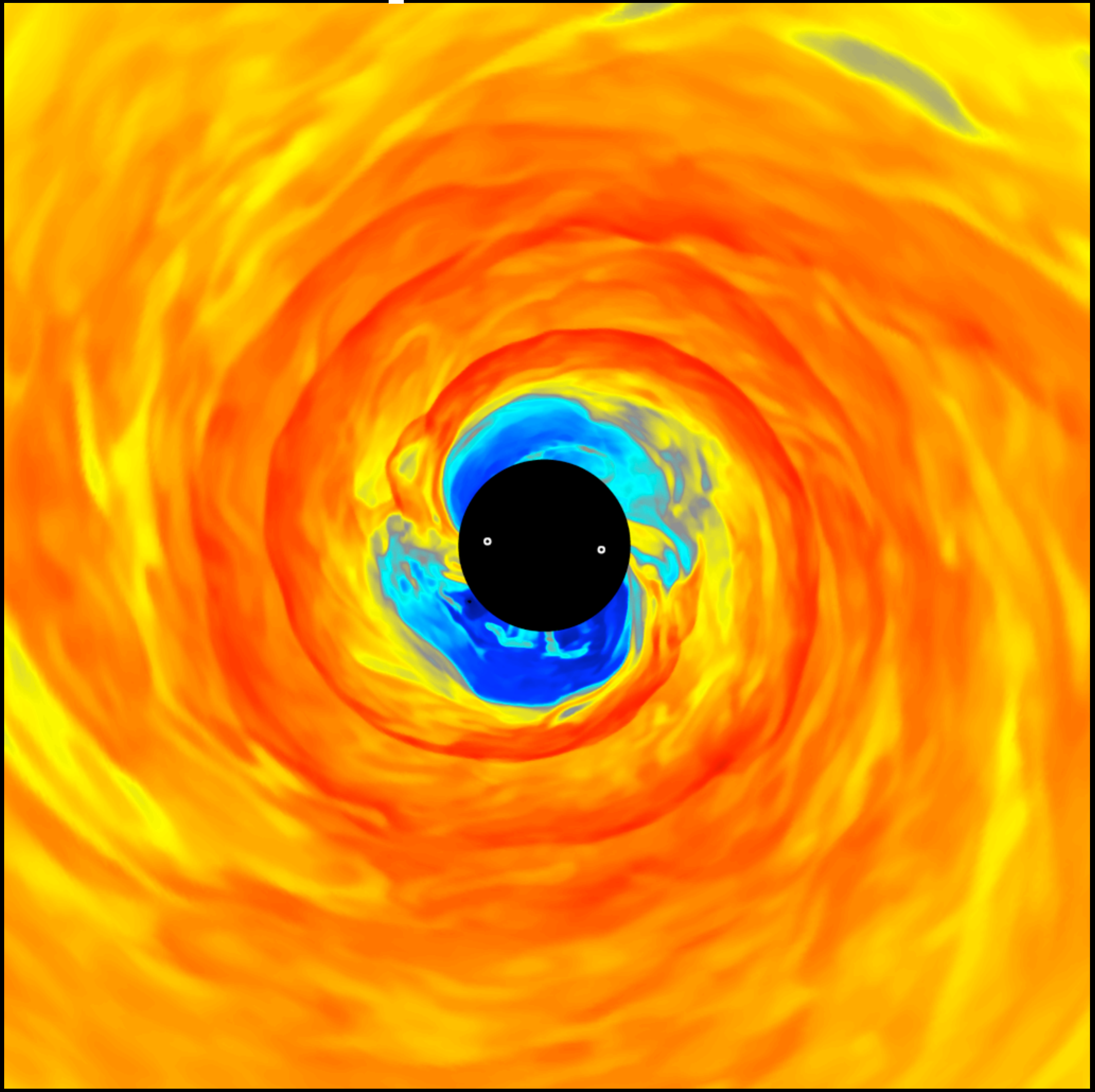
Computational Relativity and Gravitation at Petascale: Simulating and Visualizing Astrophysically Realistic Compact Binaries



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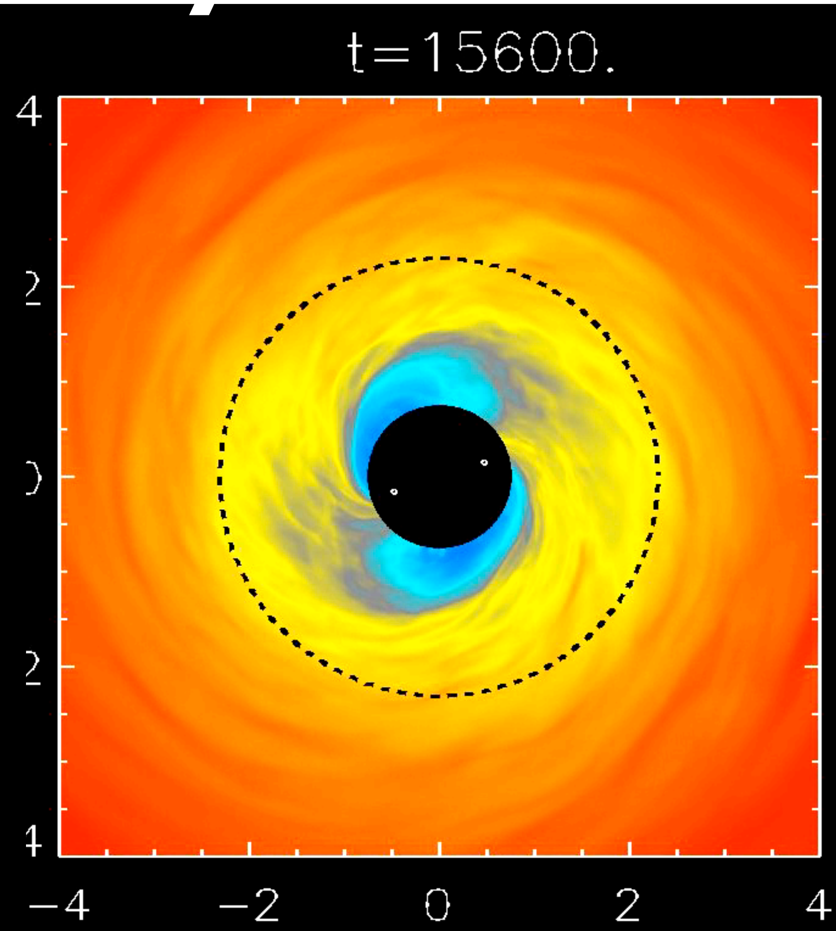
NEIS-P^2 Symposium * Blue Waters * NCSA * May 21, 2013

Circumbinary Accretion Problem:

Hopkins, Hernquist, Springel et al.



Noble++2012

Farris++2011

Physical Time (not to scale) →

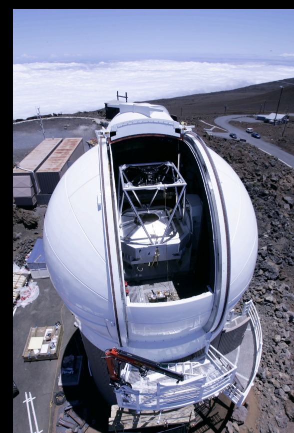
Galactic Merger	Binary Formation	Inspiral	Merger	Re-equilibration

Other Codes → Zeus → Harm3d → ET/Lazev → Harm3d

Harm3d, ET/Lazev, Harm3d ↓ Bothros

Multimessenger Synergy

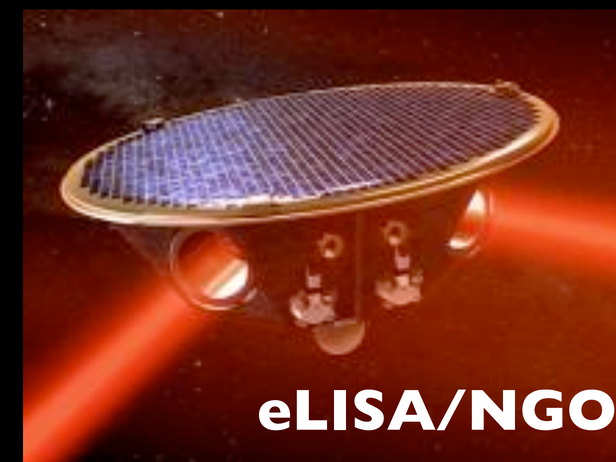
Electromagnetic Surveys



Pan-STARRS:
- 2010-??
- 4 skies per month

Large Synoptic Survey Telescope (LSST):
- 2021-2032
- 1 sky every 3 days

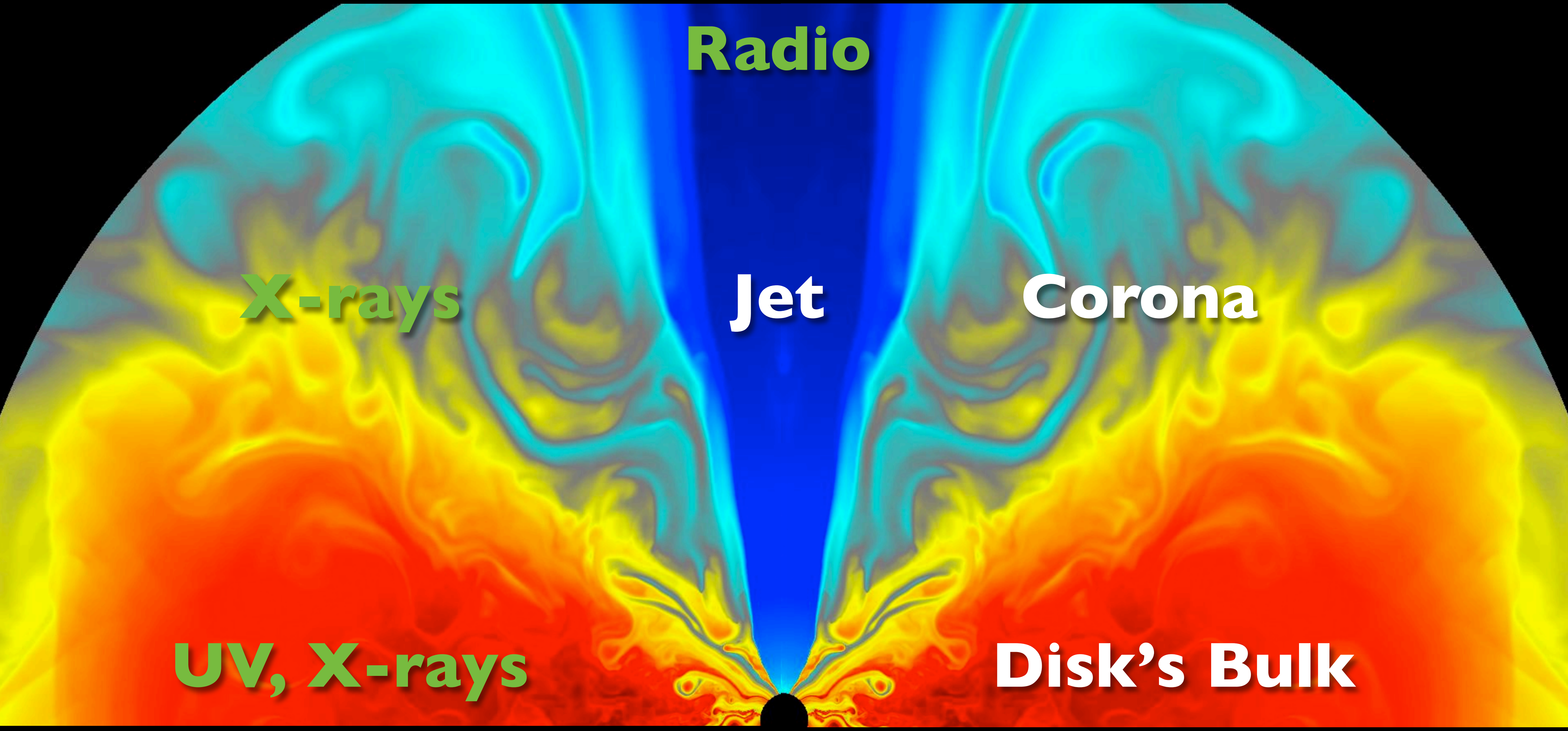
Gravitational Wave Observatories



- GW Detection/Localization <---> EM Detection/Localization;
- GW and light are connected theoretically but originate in wholly different mechanisms
  - --> independently constrain models;
- Either GW or EM observations of close supermassive BH binaries would be the first of its kind!
- Follow up (X-ray, sub-mm) observations can often be made via coordinated alert systems;
- Cosmological "Standard Sirens": New Distance vs. Redshift Measurement

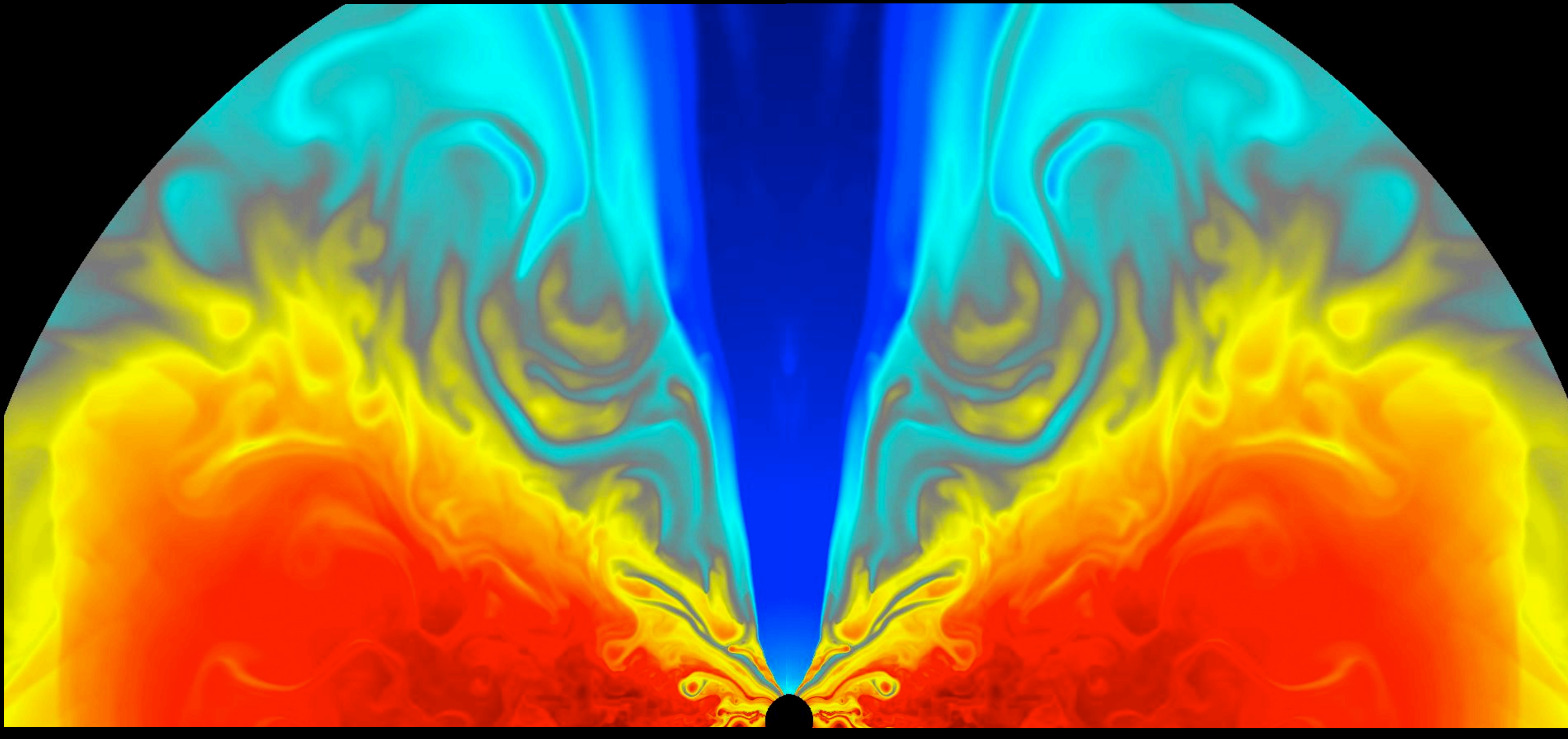
  Schutz 1986, Chernoff+Finn 1993, Finn 1996, Holz & Hughes 2005

Black Hole Accretion Anatomy



Black Hole Accretion Anatomy

- Ideal Magnetohydrodynamics (MHD)
- General Relativity (GR)
- Radiative Transfer, Ray-tracing
- Multi-species thermodynamics



The Codes

Harm3d

- **Ideal-MHD on curved spacetimes (does not evolve Einstein's Equations)**
- 8 coupled nonlinear 1st-order hyperbolic PDEs ; 1 constraint eq. (solenoidal): Constrained Transport, FluxCT method;
- Finite Volume, methods, Lax-Friedrichs, HLL fluxes (approx. Riemann solvers); PPM reconstruction; "Method of Lines": 2nd-order Runge-Kutta;
- "Mesh refinement" via coordinate transformation: Eqs. are solved on uniform "numerical" coordinates related to "physical" coordinates via nonlinear algebraic expressions;
- **Parallelization via uniform domain decomposition; 1 subdomain per process**
- **No threading, simple MPI distribution;**
- **Computationally & memory access "intensive", little I/O and MPI overhead;**
- **O(10^7 - 10^8) cells evolved for O(10^6) time steps;**

Bothros

LazEv & Einstein Toolkit

The Codes

Harm3d

Bothros

- **Predict electromagnetic emission from relativistic gas simulations;**
- Solves the Radiative Transfer and Geodesic Equations in curved spacetimes;
- RT Eq: 1 nonlinear ODE; Geodesic Eqs: 8 coupled linear ODEs;
- Post-processes Harm3d simulation data;
- $O(10^3)$ time frames of $O(10^5)$ rays that travel through 4D data cube of $O(10^{10})$ spacetime points from which O(10) functions are interpolated onto light ray's path;
- **Very Data (I/O) Intensive -- processes Terabytes of data!**
- **Originally trivially parallelized, i.e. no MPI or OpenMP support;**
    - **--> Many redundant disk reads!**

LazEv & Einstein Toolkit

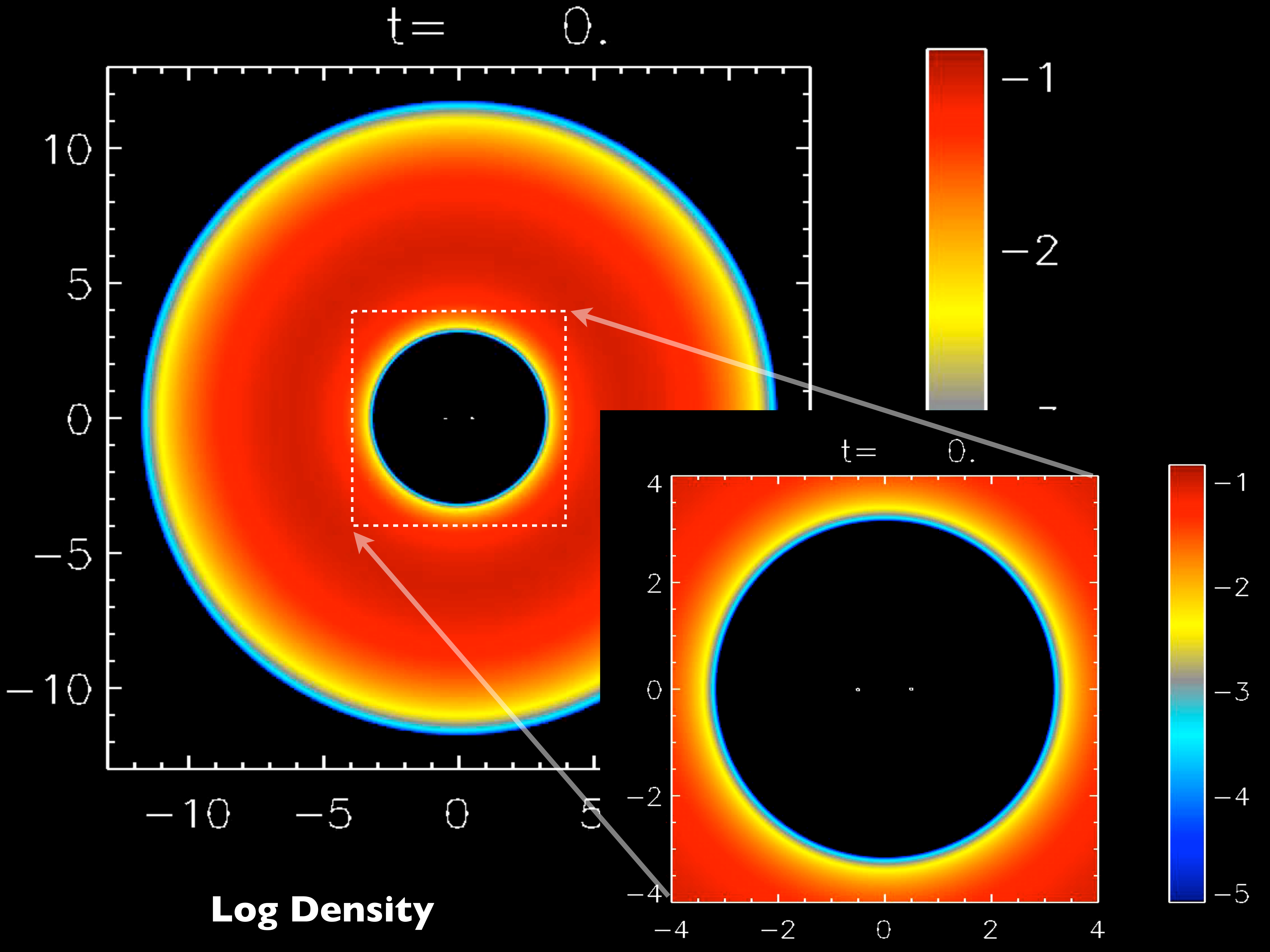
The Codes

Harm3d

Bothros

LazEv & Einstein Toolkit

- **ET = "an open, community developed software infrastructure for relativistic astrophysics";**
- Comprised of Cactus, Carpet, Whisky, McLachlan, (parts of Harm3d);
- E.g., solves Einstein's equations, w/ or w/o Hydro/MHD;
- **Block structured adaptive mesh refinement;**
- www.einsteintoolkit.org
- **LazEv = RIT's unique set of "thorns" that formulate and discretize Einstein's equations;**



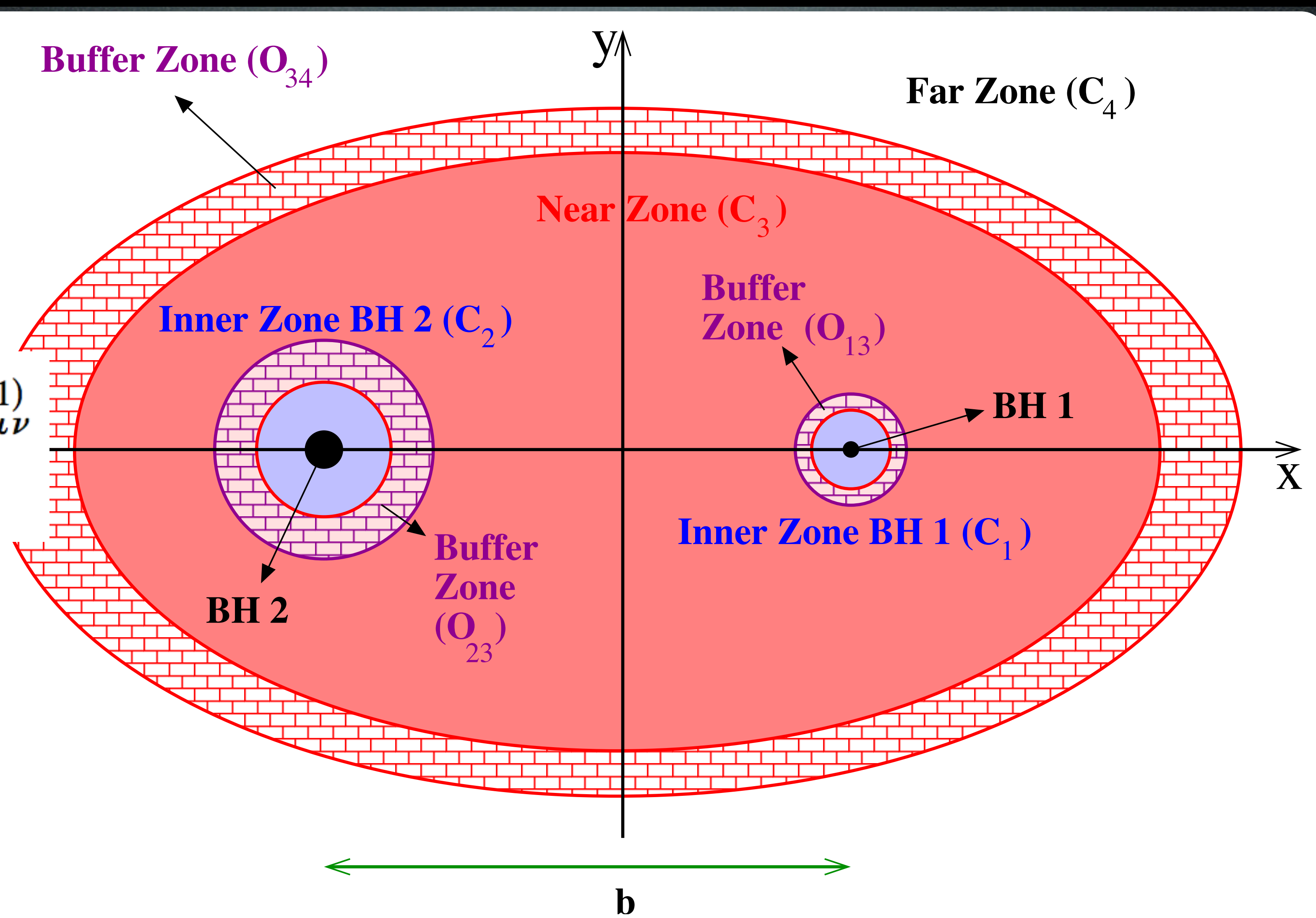
t= 0.
10
5
0
−5
−10
−10
−5
0
5
−1
−2
t= 0.
4
2
0
−2
−4
−4
−2
0
2
4
−1
−2
−3
−4
−5
Log Density

Approximate Two Black Hole Spacetimes

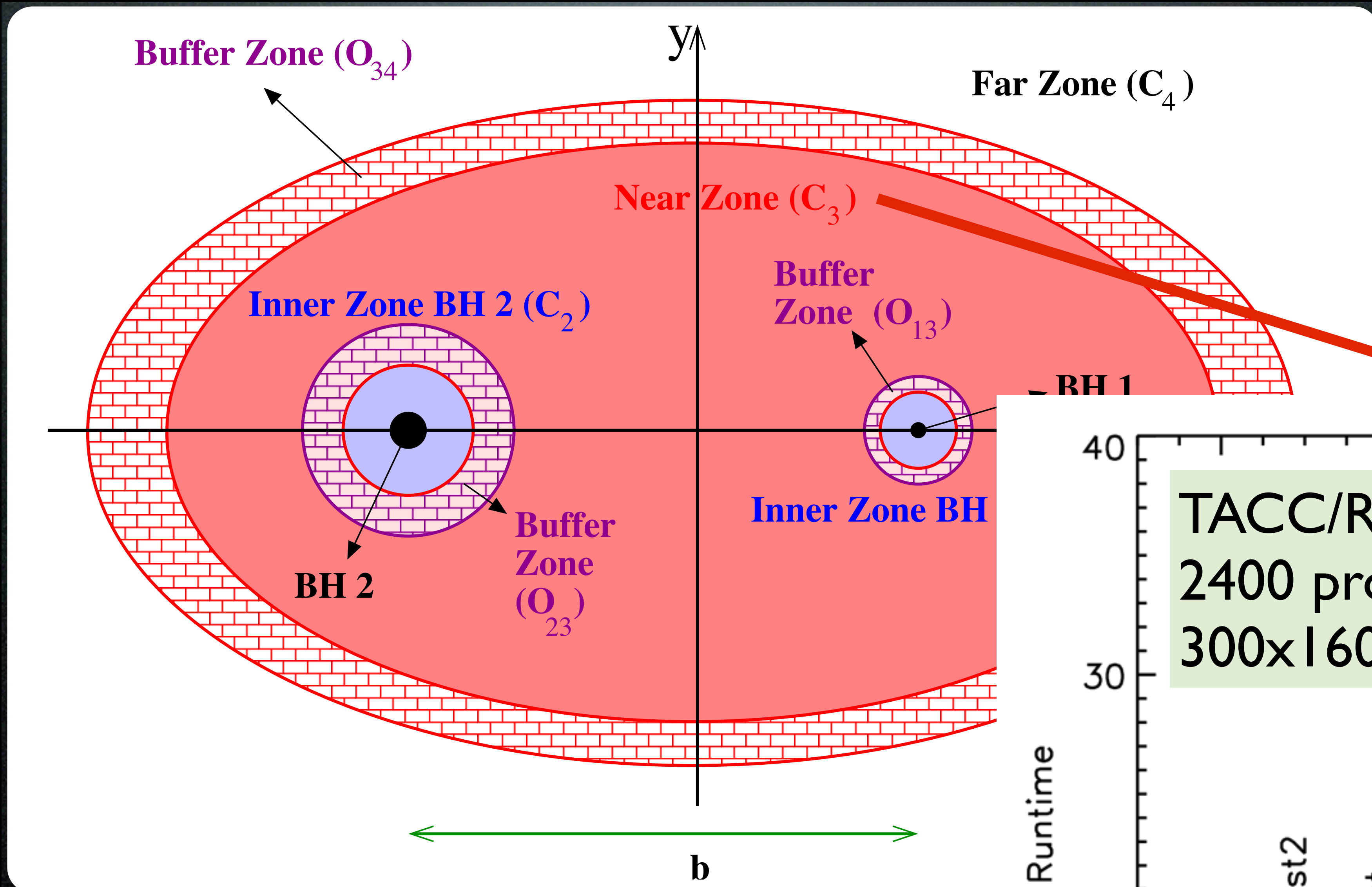
Yunes++2006, Mundim++2013

- Solve Einstein's Equations approximately, perturbatively; $\epsilon_i = m_i/r_i \sim (v_i/c)^2$
- Used as initial data of Numerical Relativity simulations;
- Closed-form expressions allow us to discretize the spacetime best for accurate matter solutions;
- Physically valid up until the last few orbits prior to merger;

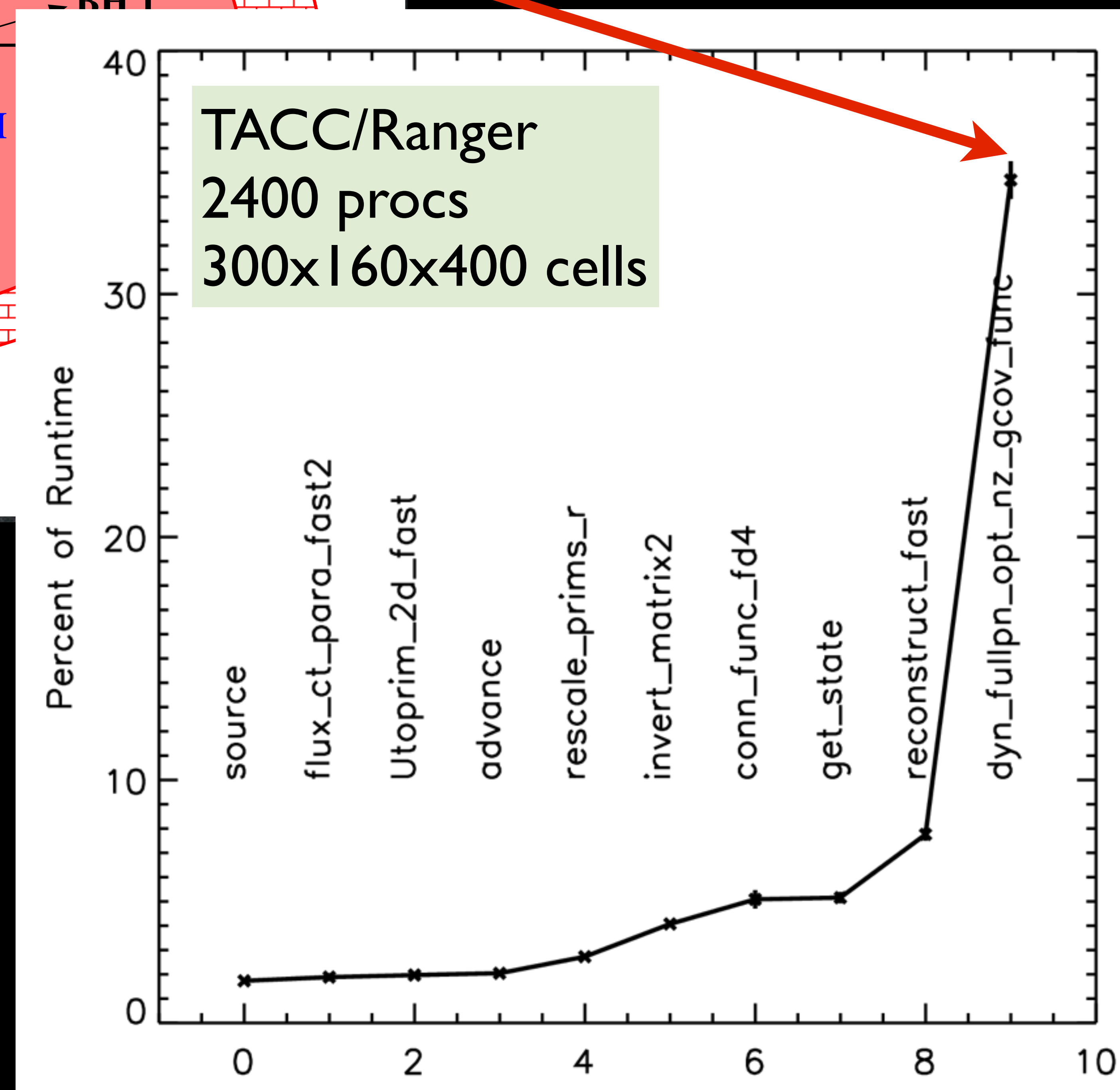
$$g^{(\mathrm{global})}_{\mu\nu} = F_2(R_2)F_1(R_1)g^{(3)}_{\mu\nu} + [1 - F_1(R_1)]g^{(1)}_{\mu\nu} + [1 - F_2(R_2)]g^{(2)}_{\mu\nu}.$$



Cost of Approximate Spacetime

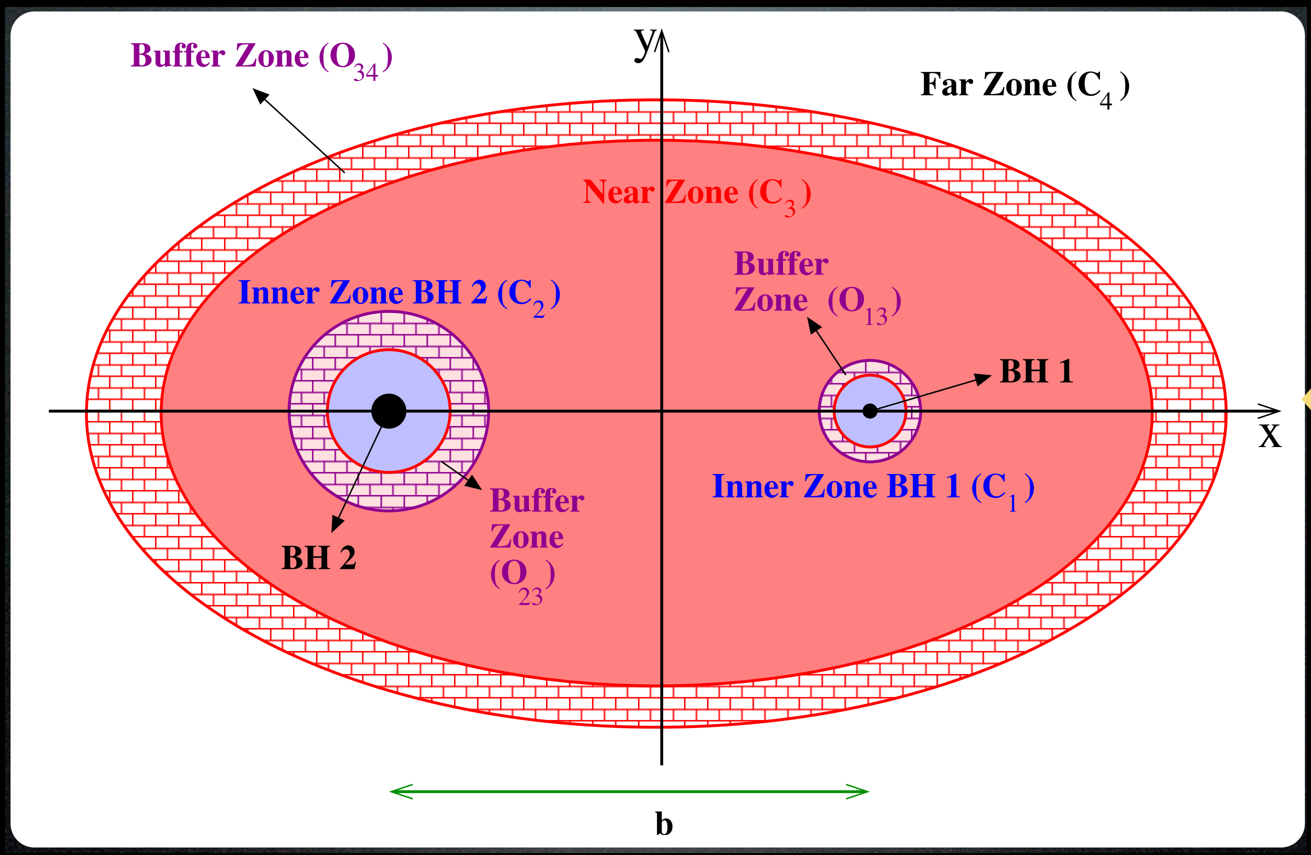


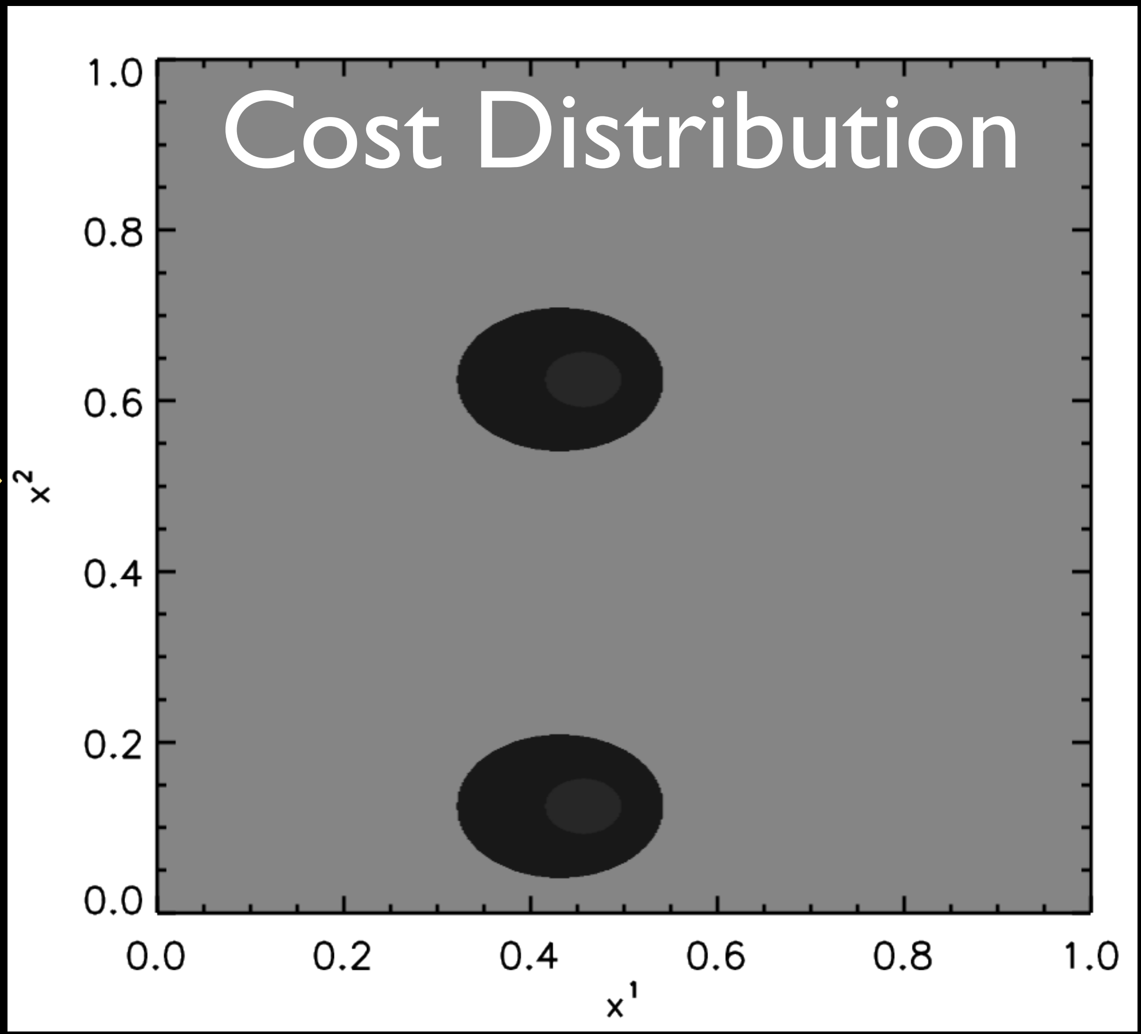
Cost of Near Zone Metric



- Significant effort spent optimizing subroutine, with the aid of symbolic manipulation software (Maple);
- Metric evaluation accounts for ~35% of runtime;

Load Balancing Domain Decomposition





- **Different zones of the spacetime vary in computational cost of evaluating metric;**
- **Strategy: decompose costlier regions into smaller domains, balancing effort across MPI processes;**
- **Black Holes (or zones) move through the grid --> "dynamic" load balancer;**
- **Need to alter static array definitions to dynamic allocations to handle nonuniform decomposition across processors;**

Zone	Relative Cost Per Cell
Inner	3
Inner/Near Buffer	4
Near	1
Near/Far Buffer	2
Far	~1

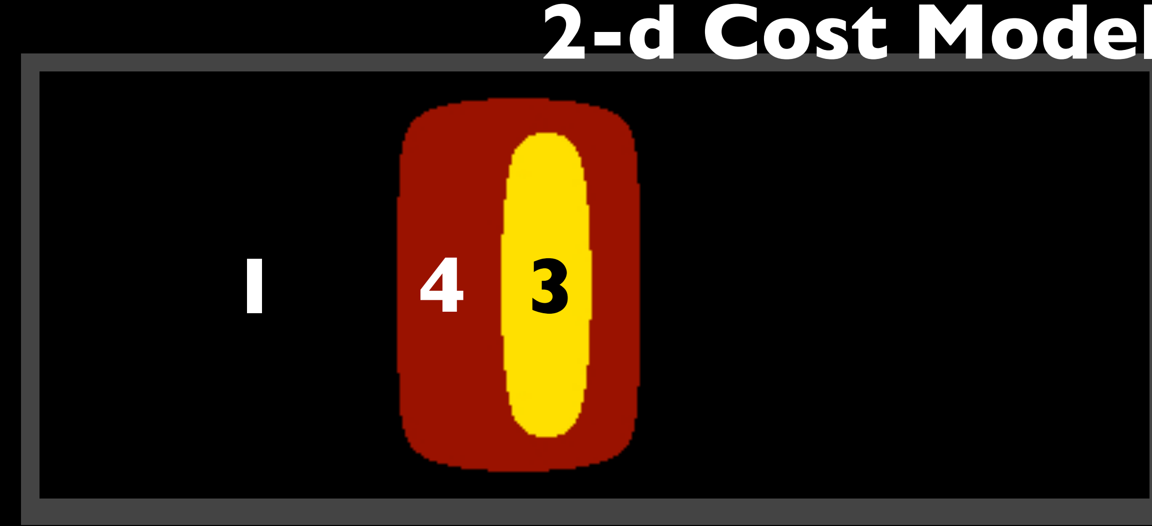
Harm3d Goals

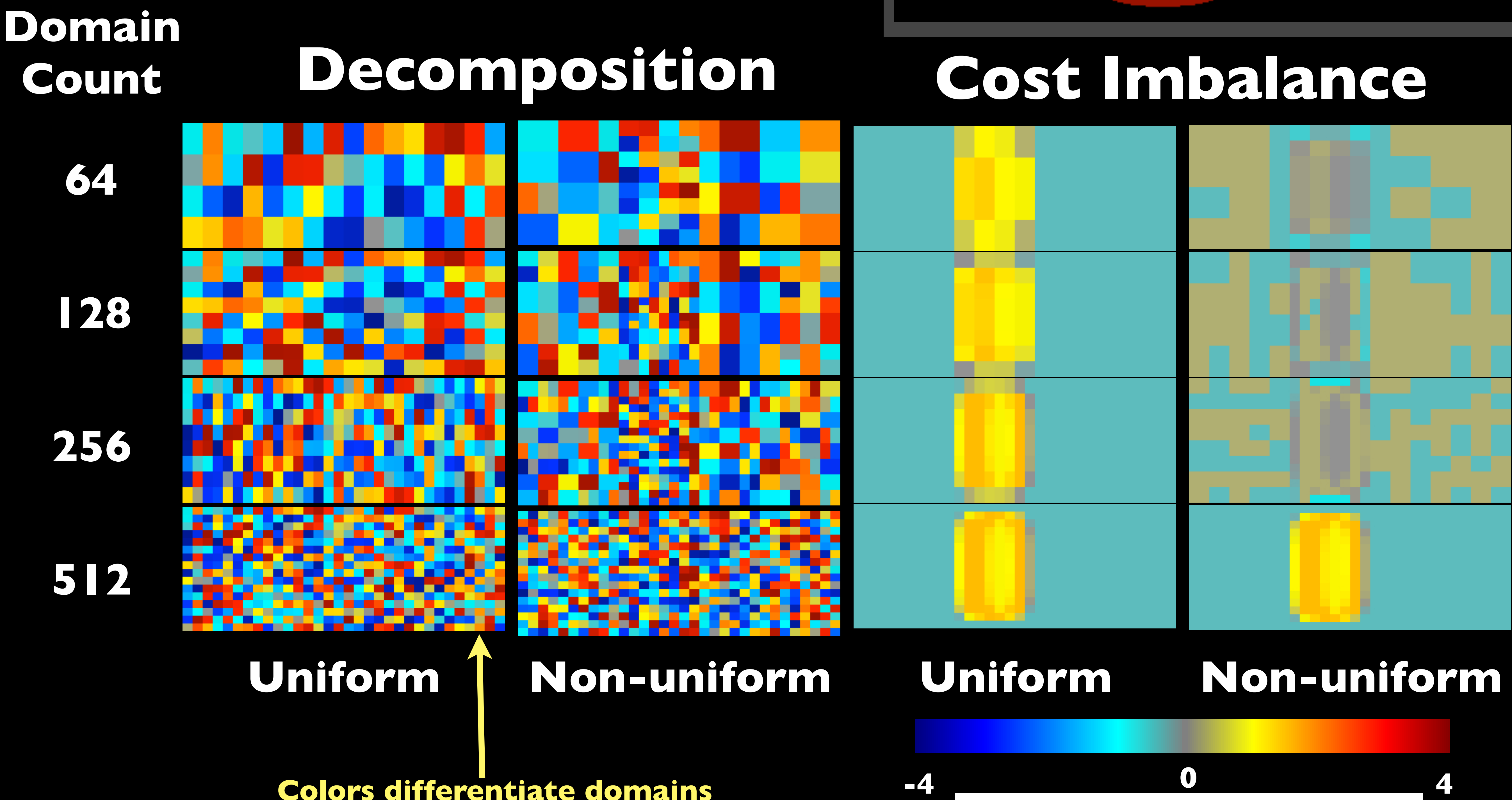
- **Solve the Load Imbalance Problem:**
  - Static Memory Allocation --> Dynamic Memory Allocation ;
  - **Nonuniform domain decomposition (different subdomain sizes across processors):**
    - Generalized subdomain boundary conditions (passing of ghost zone data);
    - Generalized data reduction routines;
  - **Load Balancing Algorithm:**
    - Method to distribute cost evenly;
    - Ability to re-evaluate cost distribution and redistribute;
  - Profile complete package on BW with a production run;
- **Incorporate OpenMP:**
  - Preliminary tests suggest only modest performance improvement;
- **May incorporate GPUs ala Jian Tao's talk & (Zink 2011)**

Load Balancing Algorithm

1. Start with global domain with cost estimates for each cell;
2. Order subdomains by cost;
3. Bisect most expensive domain along longest extent (maintain cubical domains);
4. Assign processor to new subdivision;
5. Determine neighbor relationships;
6. Repeat Steps 2 - 5   until all processors have been assigned;

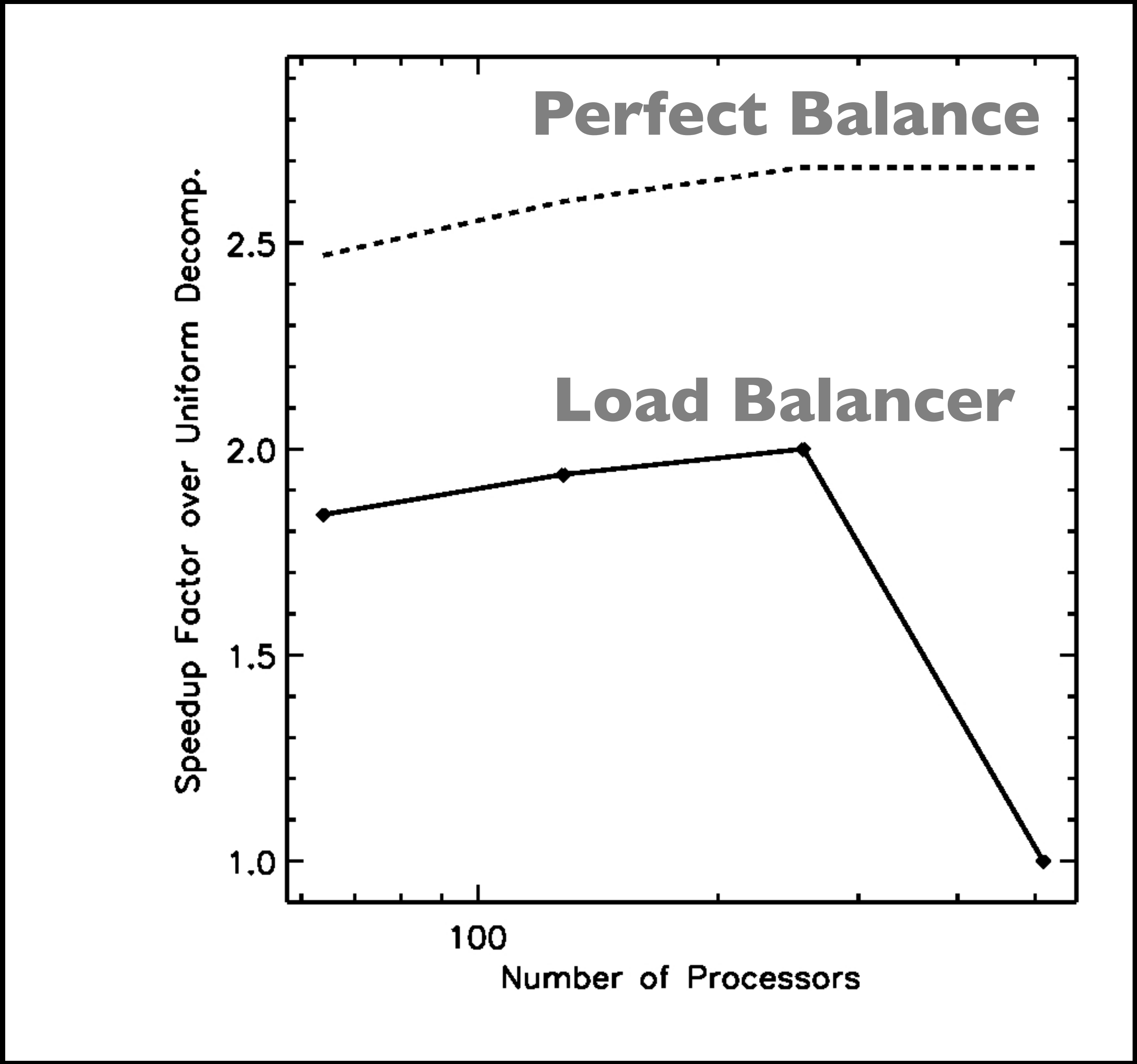
Validation of Load Balancer through Simulated Cost Distribution:



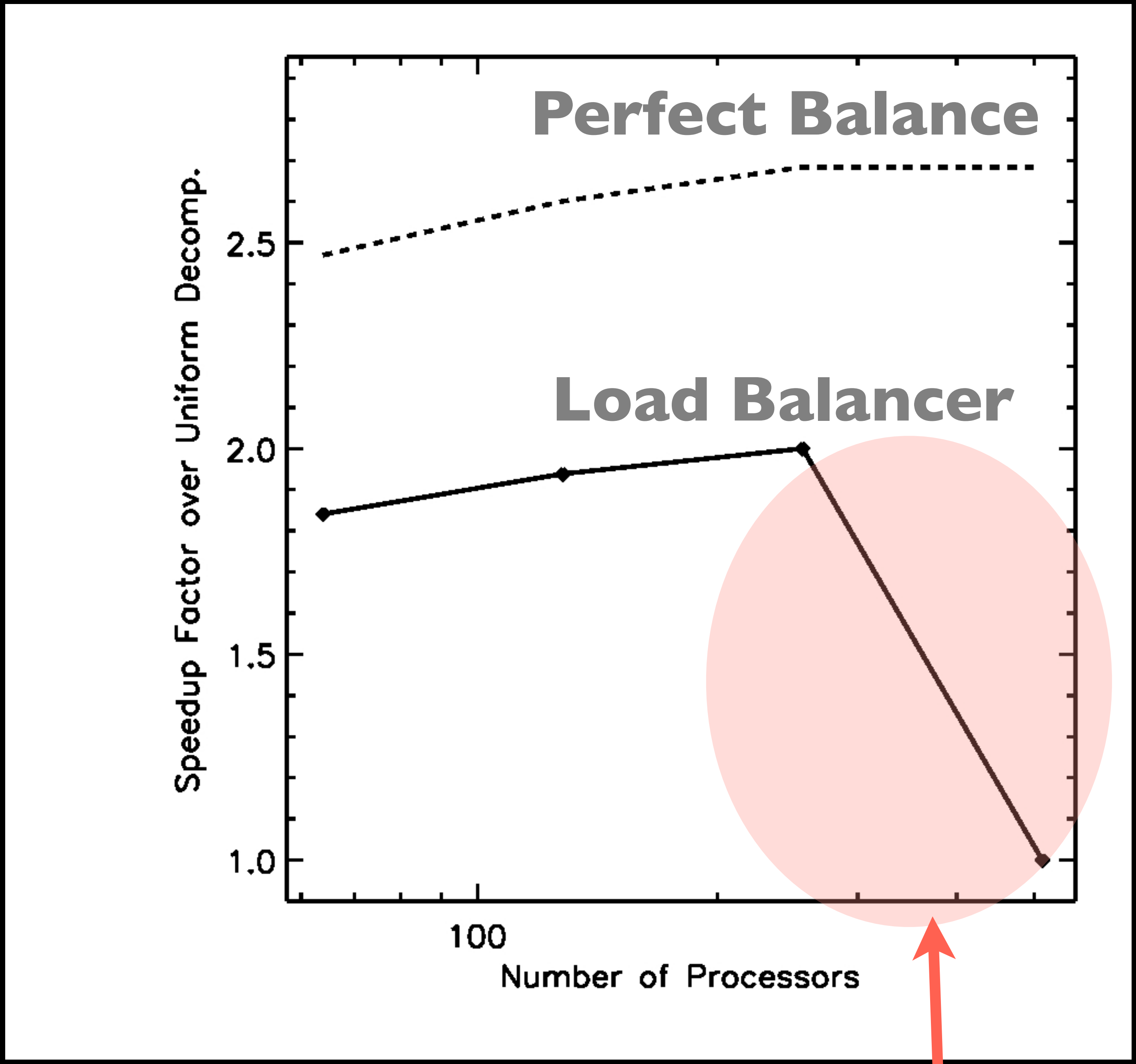


Cost Imbalance = $R_i = \dfrac{C_i - \bar{C}}{\bar{C}}$

Validation of Load Balancer through Simulated Cost Distribution:



Validation of Load Balancer through Simulated Cost Distribution:

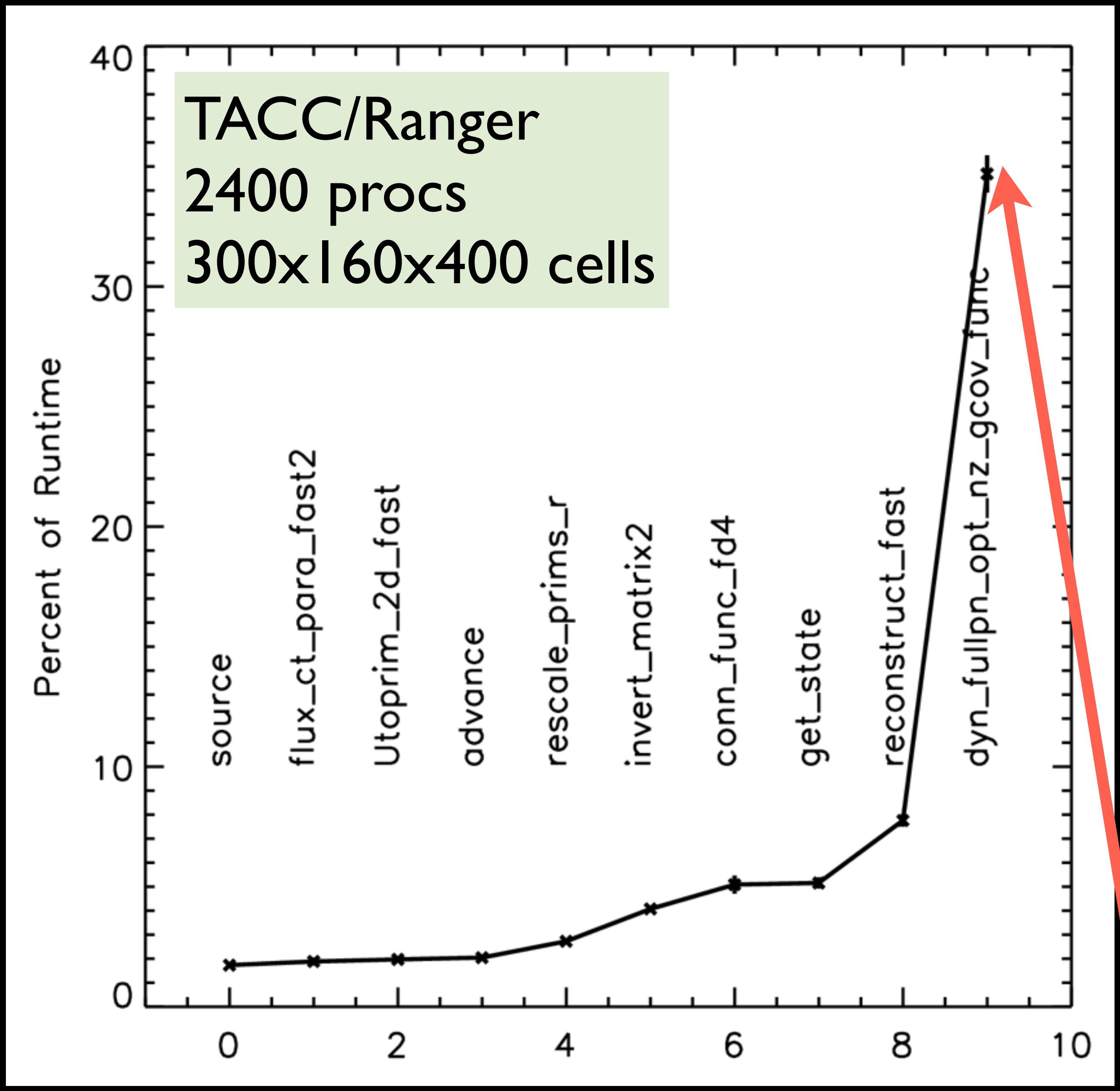


Saturation of Domain Decomposition

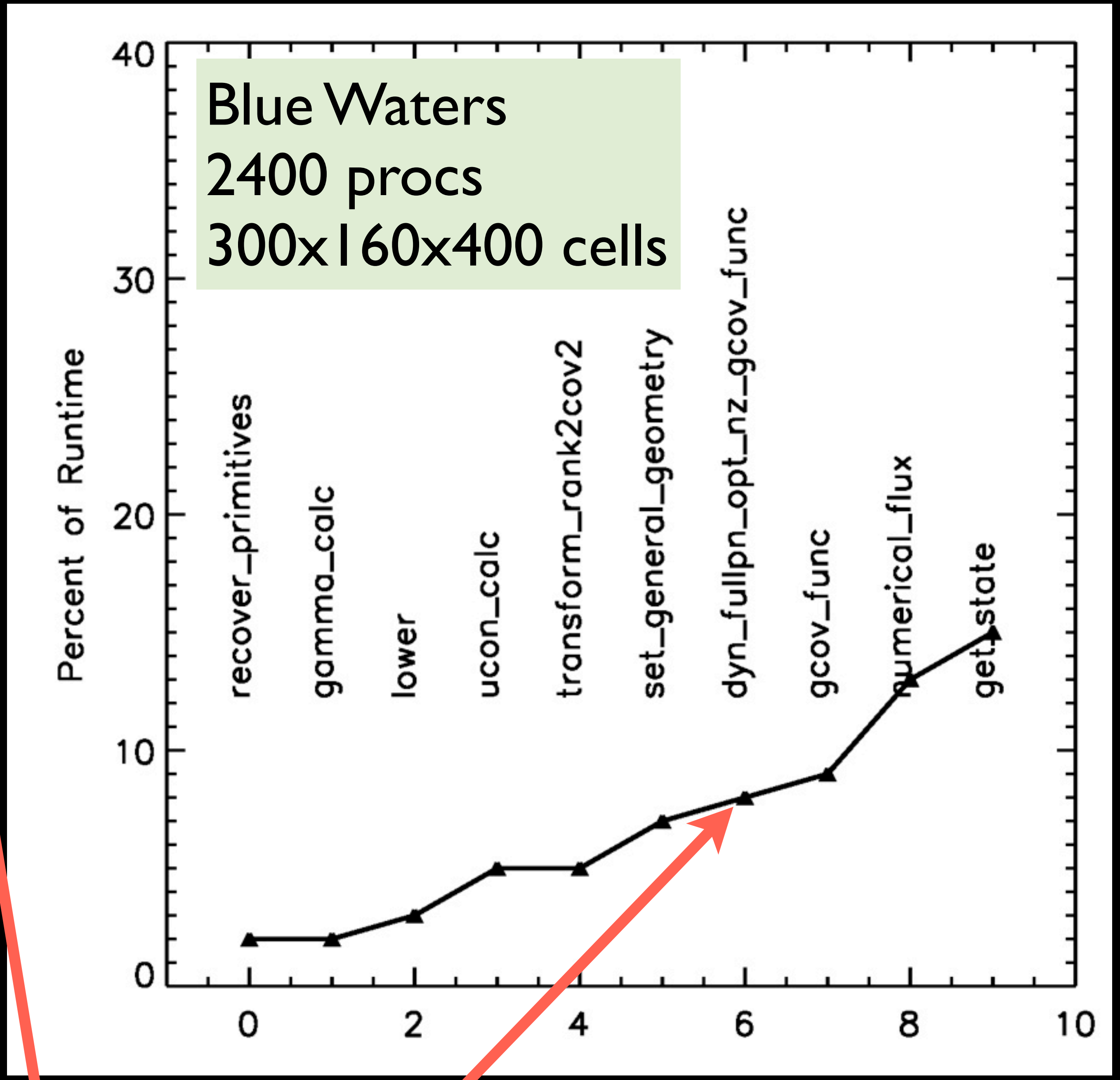
--> In practice, more processors will not be added at saturation point

Performance on Blue Waters :

Runtime Efficiency



gprof

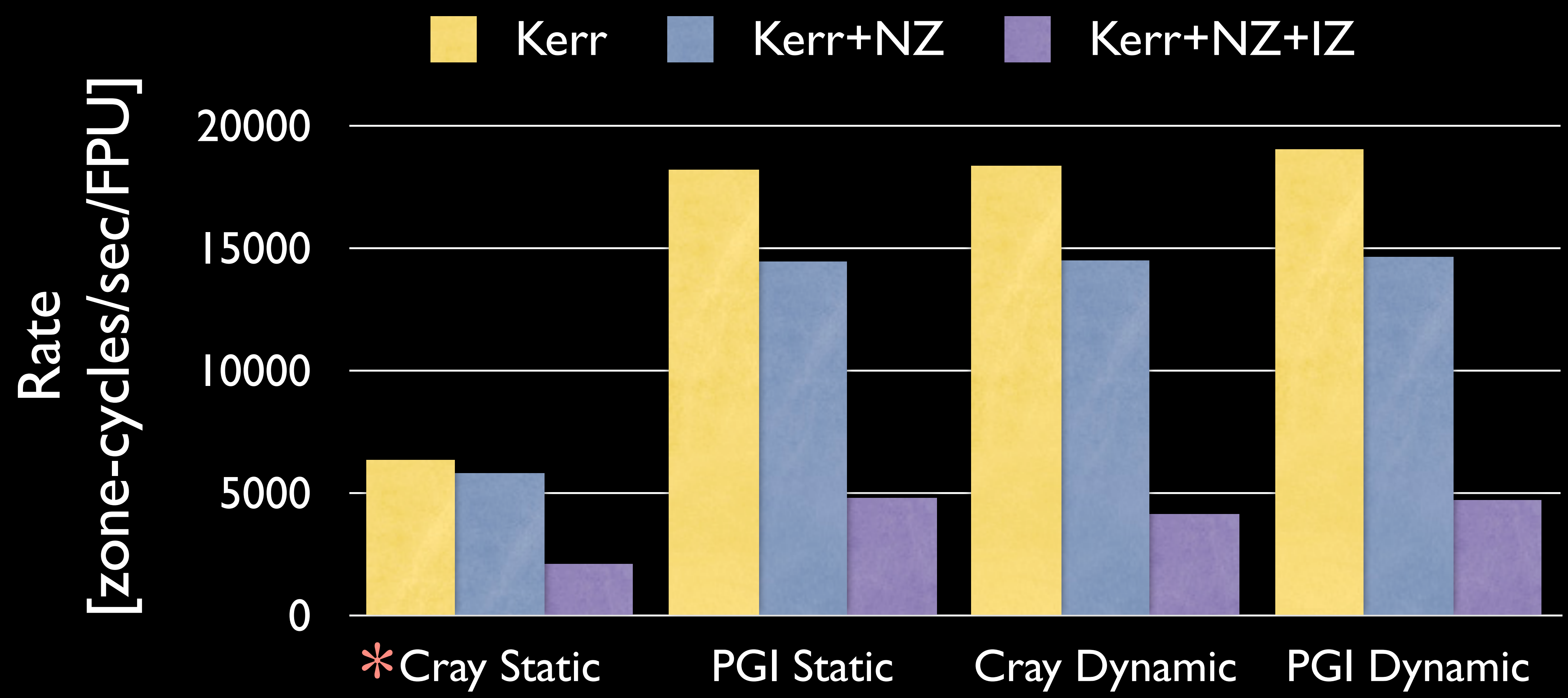


CrayPat

Why the difference?

Performance on Blue Waters :

Runtime Efficiency



* Static code seg. faults with Cray's default optimizations;

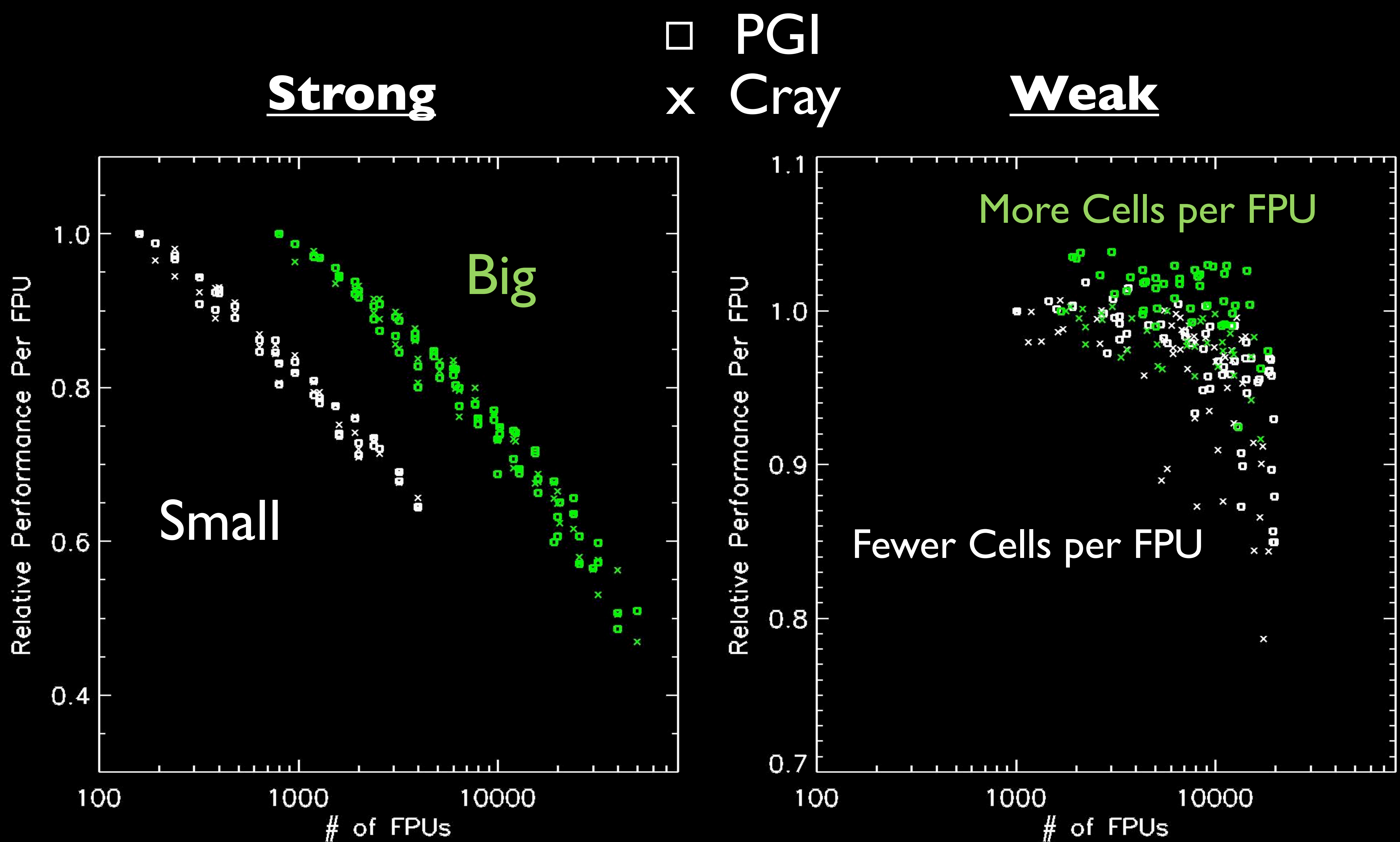
•Static = statically allocated grid functions;
•Dynamic = dynamically allocated grid functions;

•Little difference between PGI and Cray compilers;
•Little difference between Static and Dynamic memory allocation;
•Decrease in rate with more zones consistent with prior profiles;

Performance on Blue Waters :

- Using Dynamic Harm3d

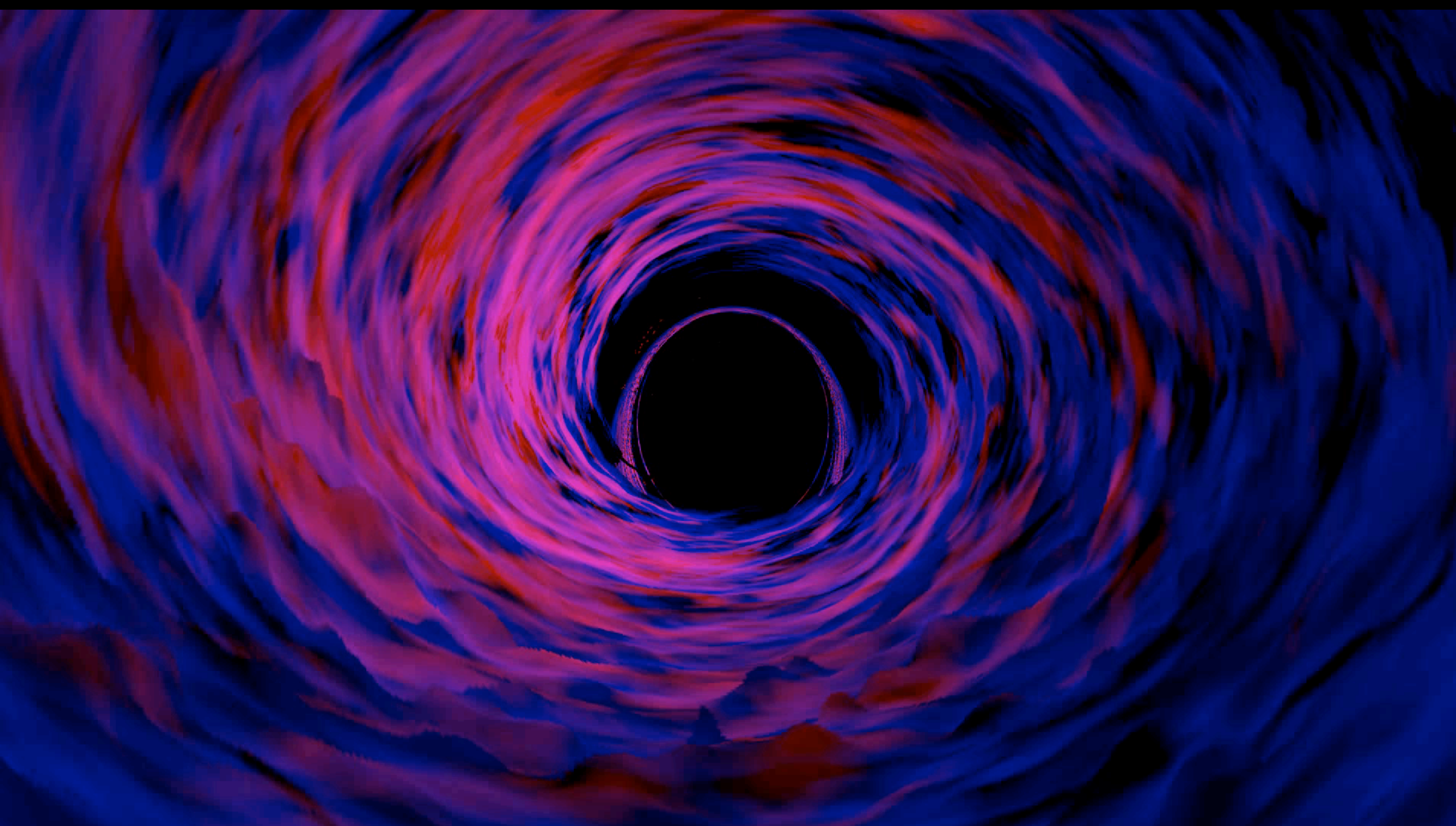
Good Scaling Performance



Bothros Goals:

Towards Radiative Transfer in Time-dependent General Relativity

- **Parallelize post-processing tool via MPI and OpenMP;**
- **Will explore how GPUs can offload effort in the future;**



X-ray Emission from Single Black Hole Disk

Noble & Krolik 2009

Schnittman, Krolik, Noble 2012

Binary Black Hole System in Photon “Cloud”

- Thesis Project of Billy Vazquez (grad student);

Bothros's Parallelization Model

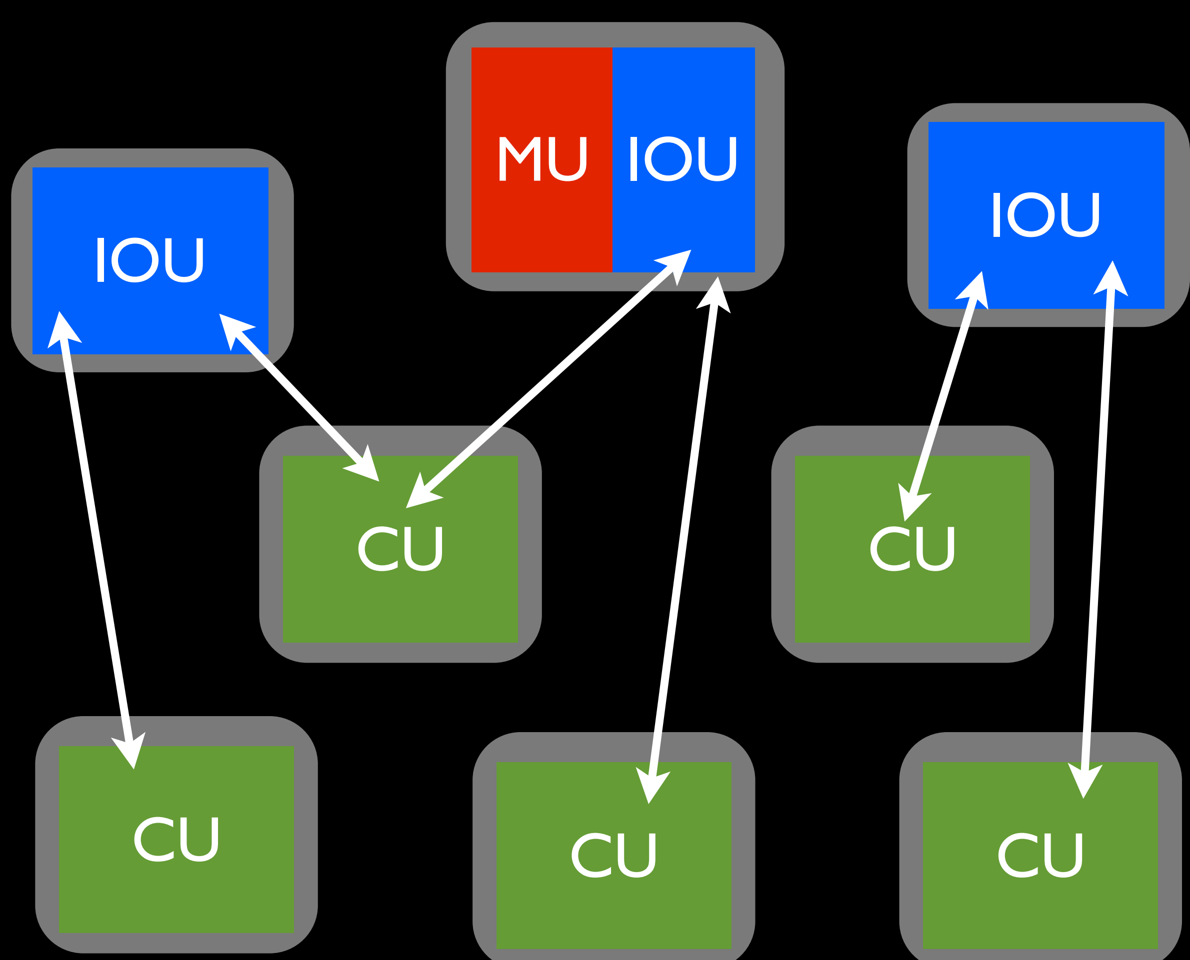
Master Unit (MU) : Evaluates problem extent; Assigns duties; Broadcasts what data is available on IOUs;

I/O Unit (IOU) : Reads time slices from disk,; Serves data to CUs when its needed, Replaces processed slices with new ones;

Compute Unit (CU) : Requests data from IOUs; Interpolate data onto rays; Integrate radiative transfer eq.; Advance rays to next data slice;

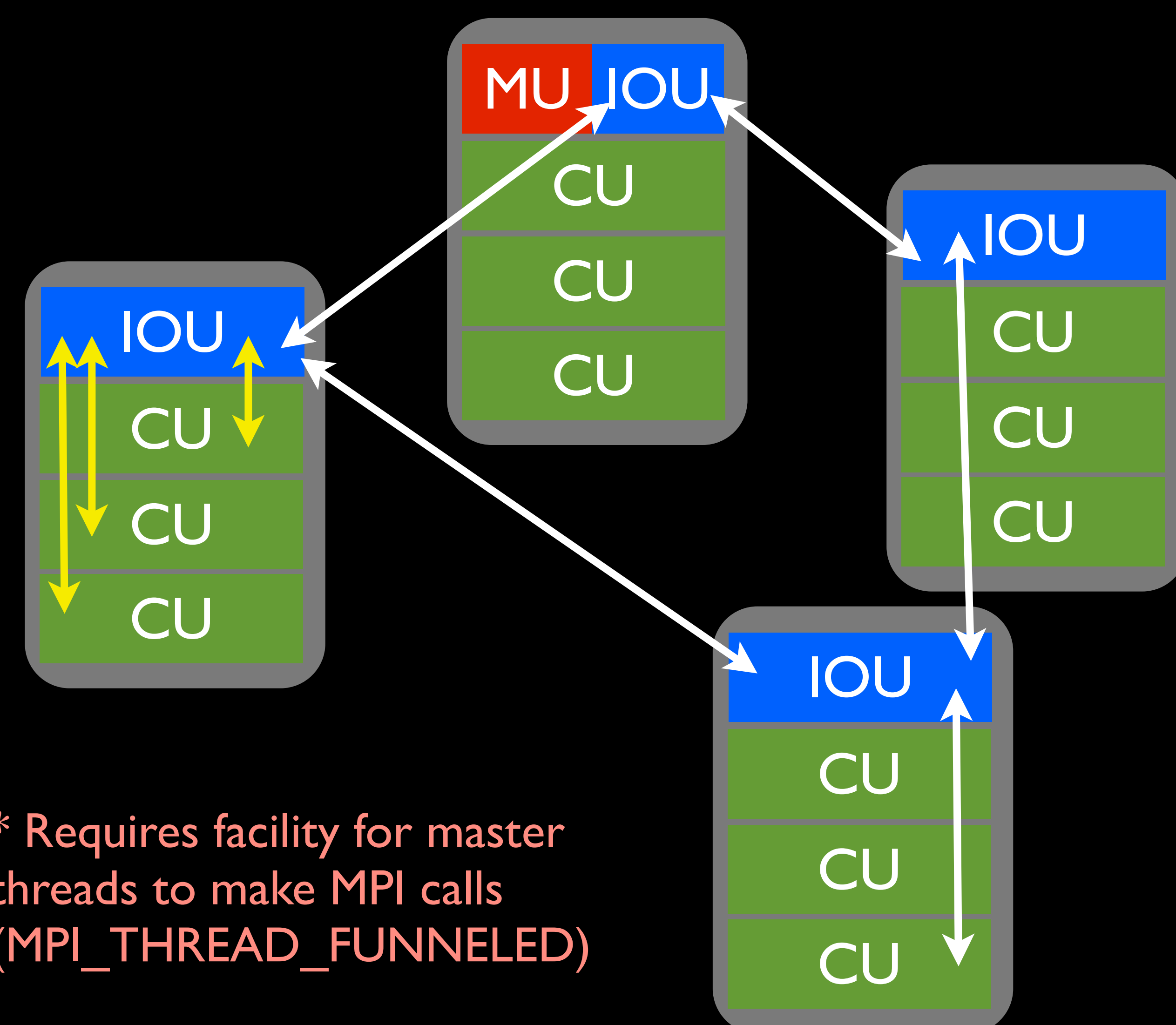
Strategy 1:

One unit per core, each threaded



Strategy 2:

One unit per thread



* Requires facility for master threads to make MPI calls (MPI_THREAD_FUNNELED)

Einstein Toolkit/LazEv Goals

- Implement threading via OpenMP throughout new GRHydro code of ET;
  - Analysis routines;
  - Reconstruction at cell interfaces;
  - Stress-energy calculation;
  - Inversion of nonlinear algrebraic equations to find primitive variables from conserved variables
- "GRHydro: A new open source general-relativistic magnetohydrodynamics code for the Einstein Toolkit", arXiv:1304.5544
- Evaluate the performance gain on Blue Waters;

Thank you to Jing Li and the rest of the support team at NCSA!!!

Conclusions:

- Blue Waters provides a singular facility and opportunity for us to calculate the most accurate electromagnetic predictions of coalescing supermassive black hole binaries;
- We are close to finishing our NEIS-P^2 version of **Harm3d**;
    - Experiments on Blue Waters confirm our earlier performance models;
    - Dynamic code scales well on Blue Waters;
    - Load balancer is expected to at least HALVE effort!
- **Bothros** development underway;
- **LazEv & Einstein Toolkit** development done, but need to profile more on BW;
- Soon, we will have circumbinary disk simulations at unprecedented accuracy, longevity, and physical realism!

Questions? Discussion....