Up to700k GPU Cores on CAS Supercomputers, for star cluster simulations around black holes

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& Silk Road Project Team
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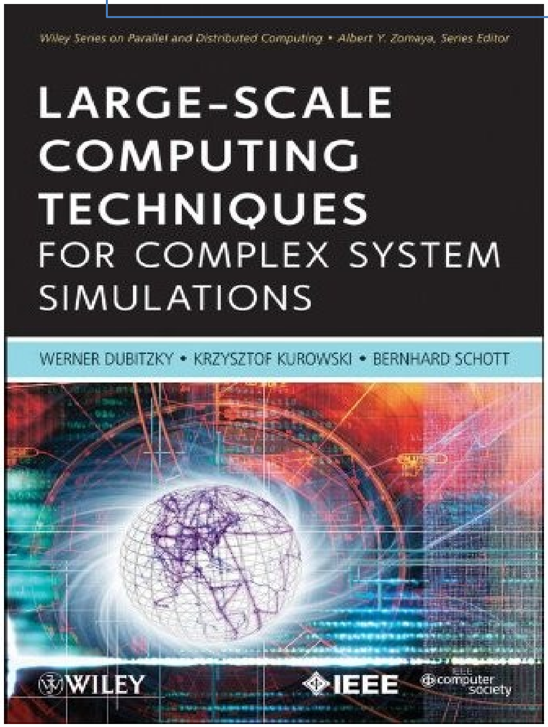
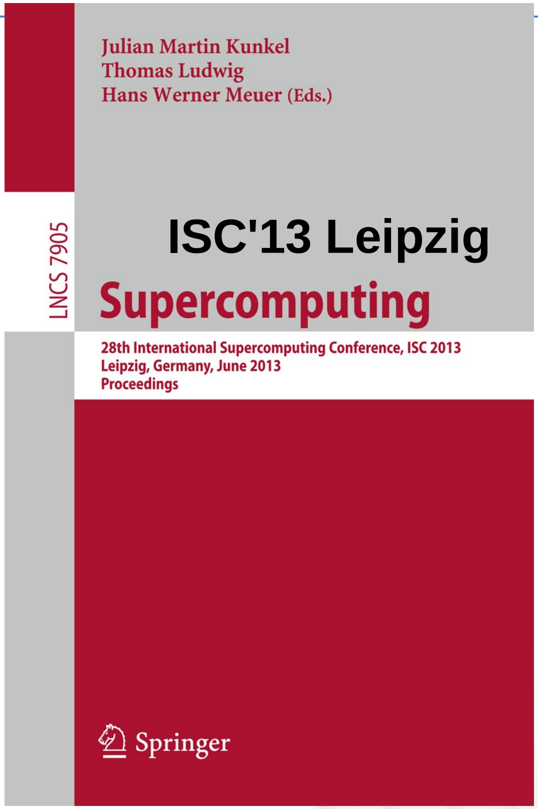
*Special State Foreign Expert in Thousand People's Plan in China

PRACE Award - 2011

Astrophysical Particle Simulations with Large Custom GPU Clusters on Three Continents

Rainer Spurzem, *et al*, Chinese Academy of Sciences & University of Heidelberg



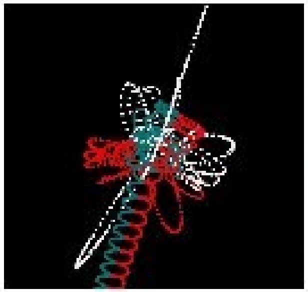
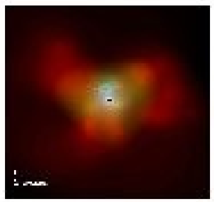


中国科学院国家天文台
NATIONAL ASTRONOMICAL OBSERVATORIES ,CHINESE ACADEMY OF SCIENCES

北京大學
PEKING UNIVERSITY

Our Main Research Projects are:

- Binary Supermassive Black Holes and Gravitational Waves in Quiet and Active Galactic Nuclei


- Dynamical Evolution of Stars and Gas in Galactic Nuclei and Dense Star Clusters
- How are planetary systems forming and evolving (in star clusters)?
- How can we design supercomputers which are faster and consume less energy?


ICCS
International Center for Computational Science

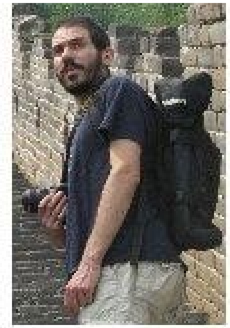
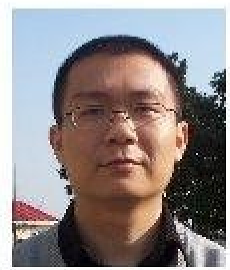
- Education and Workshops in Computational and Theoretical Astrophysics, Parallel Programming and Accelerated Computing

中国科学院国家天文台
National Astronomical Observatories, CAS

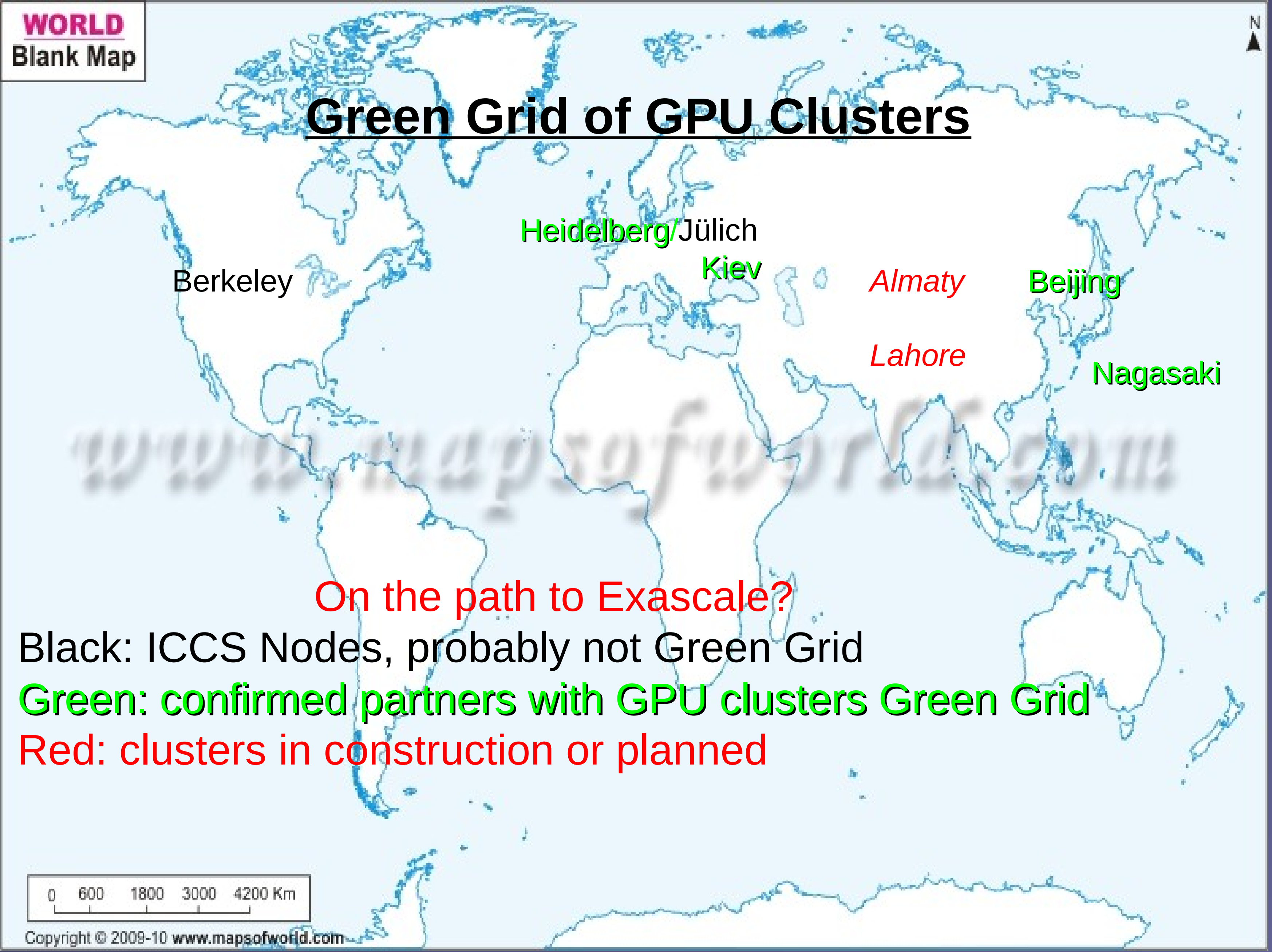
the SILK ROAD PROJECT at NAOC
丝绸之路 计划

Team

	Name and Position	Research Interests
	**Rainer Spurzem** CAS Visiting Professor, Senior International Scientists Professor at Heidelberg University (on partial leave)	Stellar Dynamics, Star Clusters, Black Holes, Galactic Nuclei, Gravitational Waves, Many Core Supercomputing and Parallel Programming
	Liu Chuan-Wu	Master Student-Star Clusters
	Peter Berczik Senior Silk Road Project Postdoc	Senior Postdoc Galactic Nuclei Computational and Hardware Expert
	Gareth Kennedy Postdoc, CAS Fellow	Stability in the three-body problem, Dynamics of globular clusters, Stellar and gas dynamics in galactic centres
	Shuo Li Postdoc	Dynamical evolution of supermassive BH / BH binaries and galactic nuclei, Gravitational waves, Computational astrophysics

	**Luca Naso** Postdoc, CAS Fellow	Accretion Physics, Compact Objects, Magnetic Fields, Numerical Astrophysics
	Shiyan Zhong	Doctoral Student Galactic Nuclei, Black H Tidal Accretion of Stars
	**Lei Liu** Graduate student at: (1) Astronomisches Rechen-Instit Zentrum fuer Astronomie, Heidelbe University and (2) National Astronomical Observatories, CAS)	Galaxy formation, numerical simulation, GPU computing
	Changhua Li	System Administrator Grid Software Expert
	Hazel Wei Administrative staff	Administrative Office Assistant

Green Grid of GPU Clusters



On the path to Exascale?

Black: ICCS Nodes, probably not Green Grid

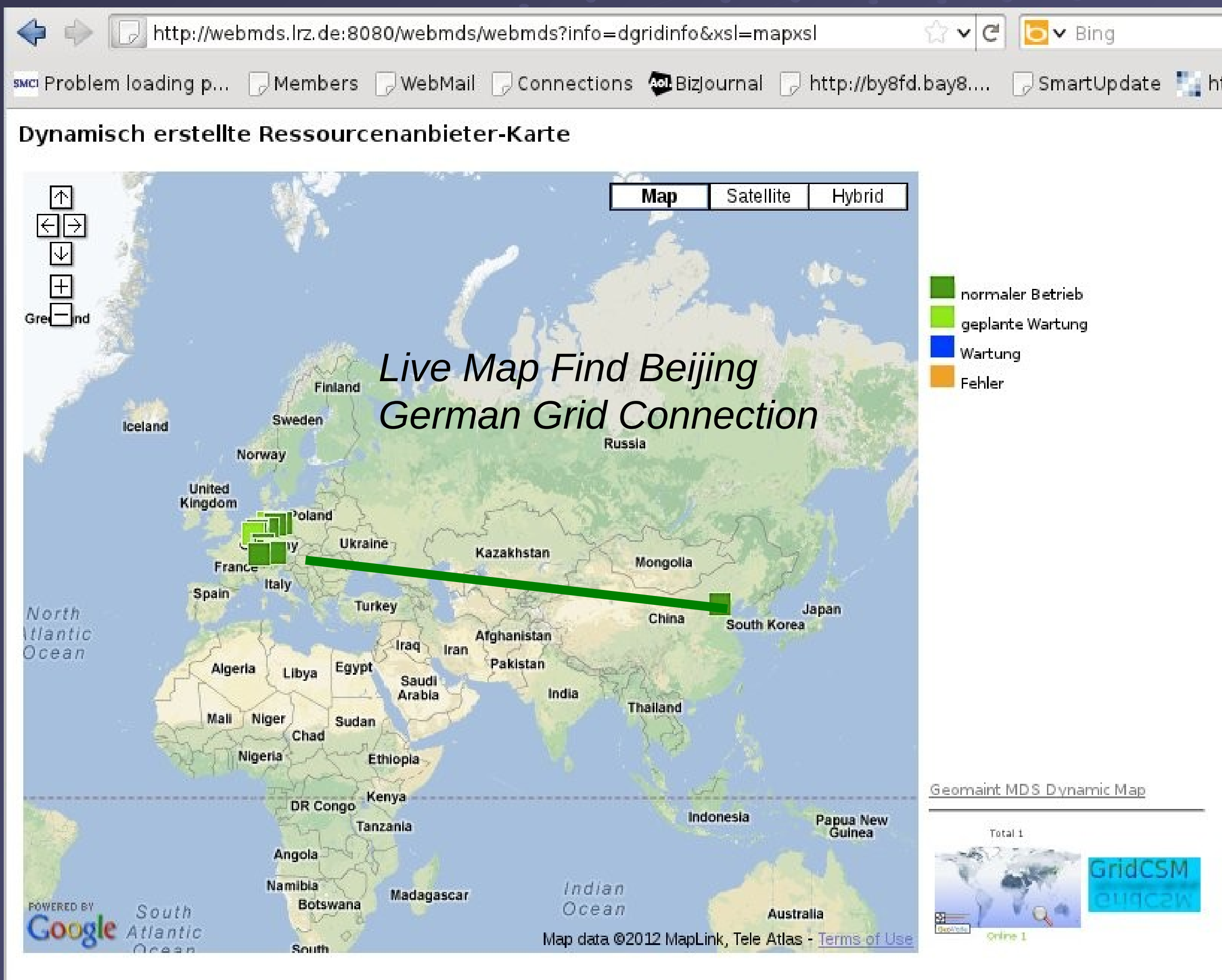
Green: confirmed partners with GPU clusters Green Grid

Red: clusters in construction or planned

Green Grid

China National Grid

http://webmds.lrz.de:8080/webmds/webmds?info=dgridinfo&xsl=mapxsl



Some Software used from:
D-Grid / Astrogrid-D = German Astronomy Community Grid

http://www.gac-grid.org

Globus GT 4.0 (soon 5.0)
Gridway Job Submission

Authentication through Root-CA;s in China (IHEP) and Germany (DFN)
Simple File Transfer

Much work in progress...

Star Clusters, Black Holes, Gravitational Waves

- Hardware accelerated
- Astrophysics: Black Holes, gravitational waves
- Software and Scaling

国家天文台 GPU 超级计算机<u>老虎</u>

性能描述： 85 个计算节点，通过 Infiniband 高速网络连接；每个节点安装了 2 个 4 核的 Xeon E5520 中央处理器， 24GB 内存， CPU 理论峰值为 1.5 万亿次；每个节点安装了 2 块 Nvidia C1060 图形加速卡，理论单精度浮点计算峰值约为 160 万亿次。

Upgrade of 老虎 Sep. 2013 – for Kepler GPU ...

59 (64) Kepler K20X GPU

1.31/3.95 Tflop/s double/single

6 GB Memory

250 GB/sec Bandwidth

2688 cores

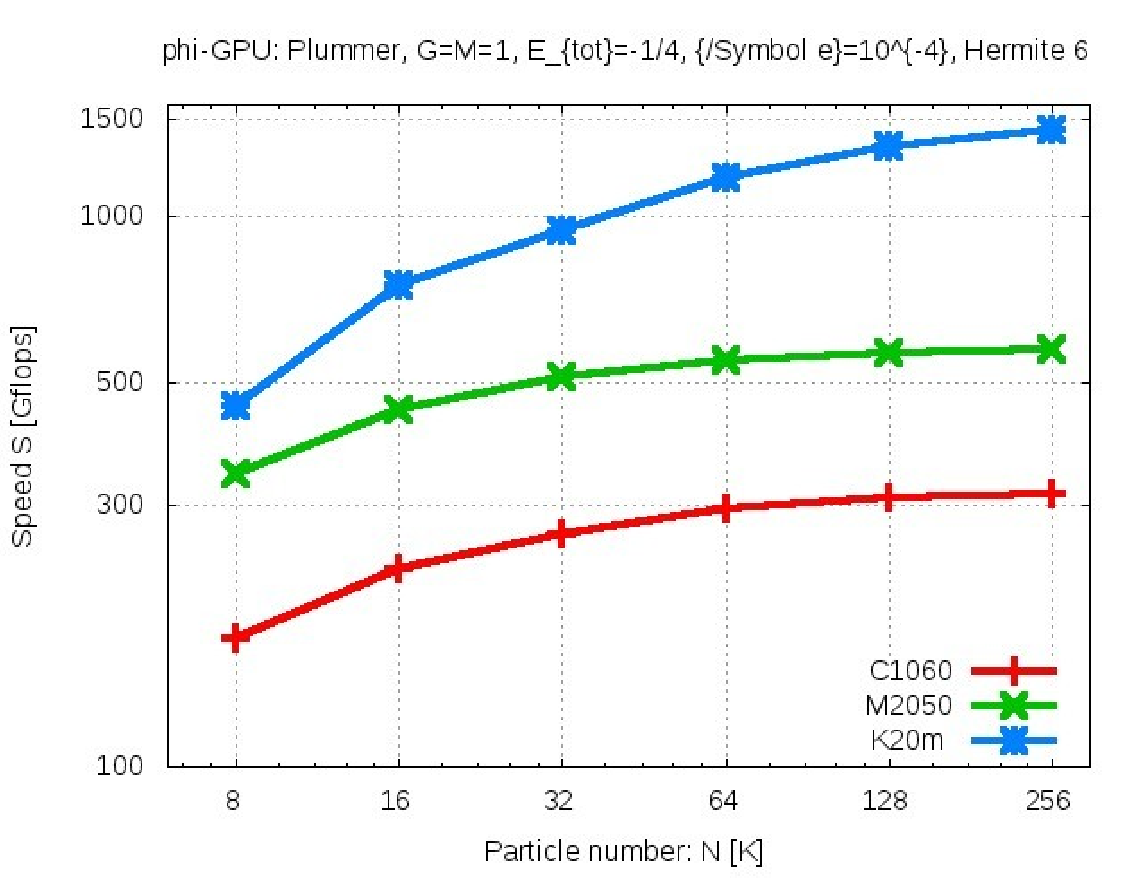
Old Tesla C1060 of 2009:

1.00 single / 0.3 double (emulated)

2 GB Memory

440 cores

Kepler Scaling, it works...



Spurzem, Berczik, et al., 2013, LNCS Supercomputing, 2013, pp. 13-25, Springer publisher.

Fig. 4. Here we report a preliminary result from a benchmark test of our code on one Kepler K20 card; we compare with the performance on Fermi C2050 (used in the Mole-8.5 cluster), and the oldest Tesla C1060 GPU (used in the laohu cluster of 2009) - the latter is used as a normalization reference. We plot the speed ratio of our usual benchmarking simulation used in the previous figures, as a function of particle number. From this we see the sustained performance of a Kepler K20 would be about 1.4 - 1.5 Tflop/s.

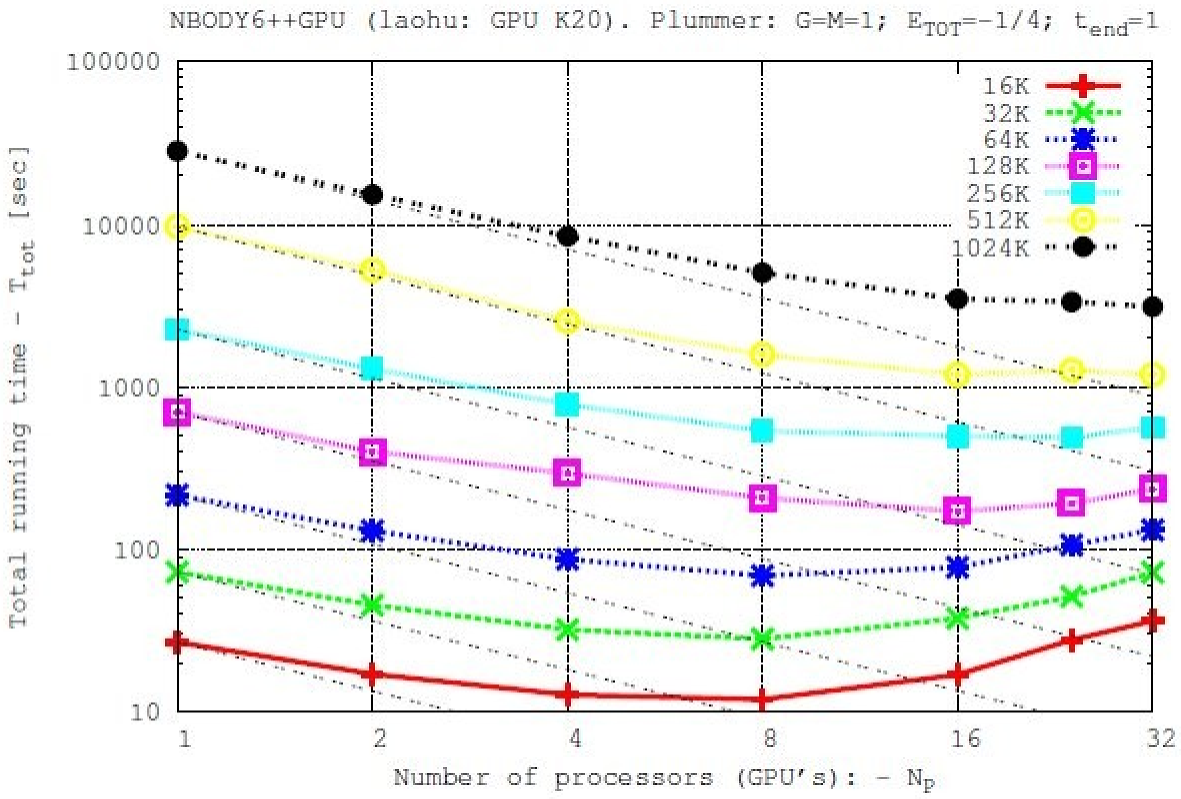


Figure 3. Total wall clock time of 1 time unit integration with the NBODY6++GPU on the K20 GPU cards. The lines with different symbols presents the different particle numbers.

Strong Scaling of Legacy Code NBODY6++ with 32 Kepler K20

on

Beijing NAOC laohu cluster

Current project 2012-2014: Milky Way + Judge at FZ Jülich, Germany

SFB 881 – The Milky Way System

Collaboration with

FZ Jülich, Germany

204 nodes ~ 2448 CPU cores

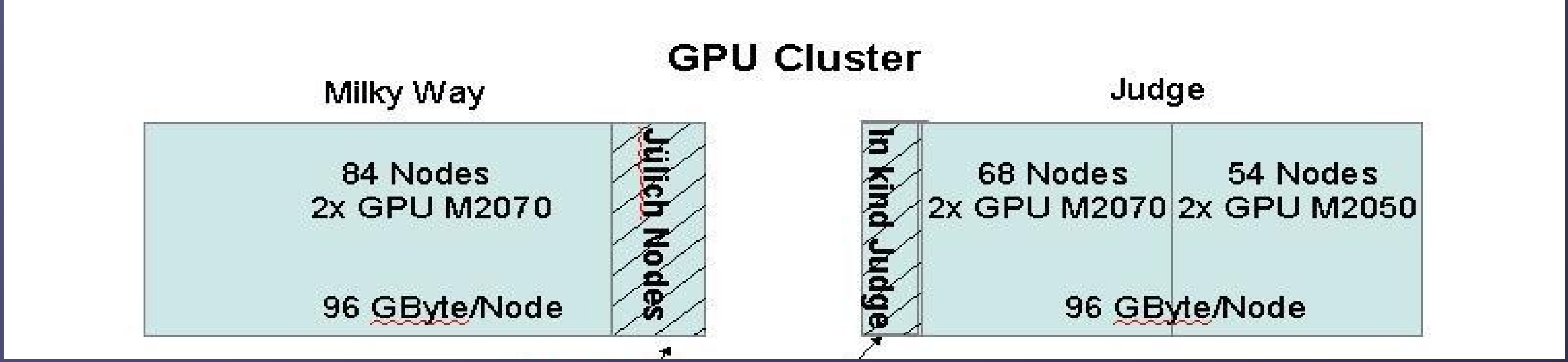
20 TB CPU memory

408 GPUs M2070/M2050

~ 200.000 GPU threads

2 TB GPU device memory

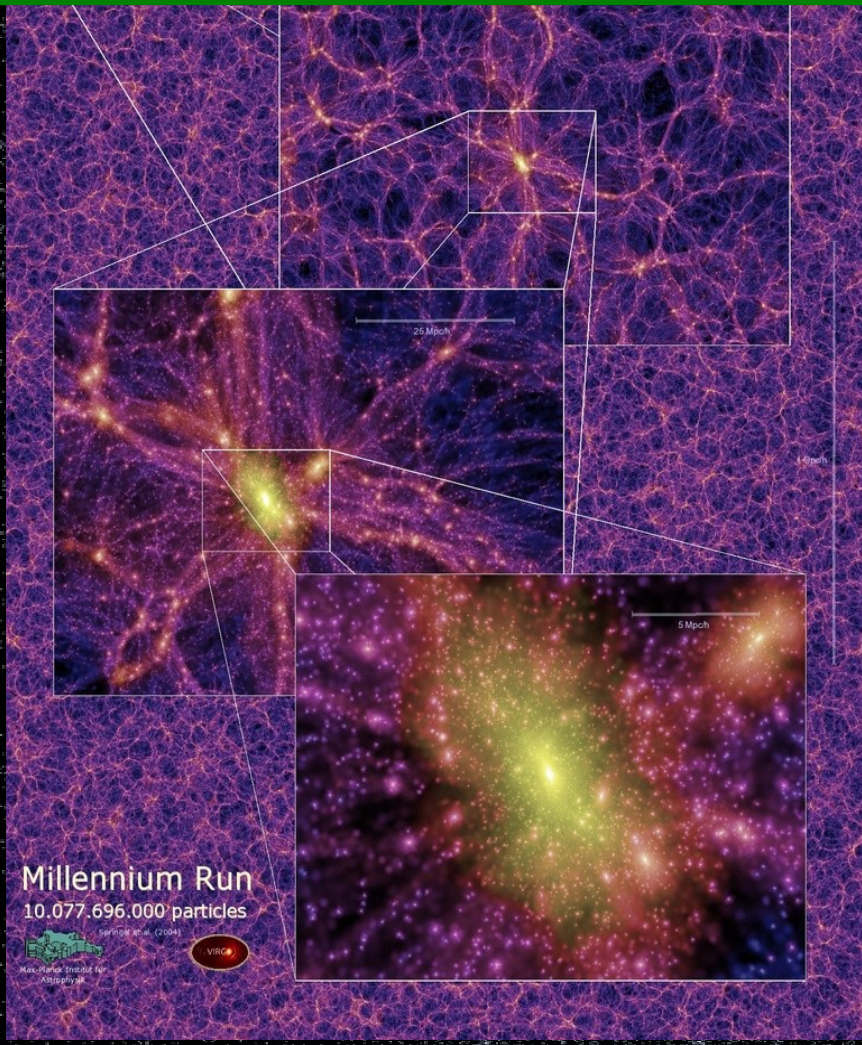
Spring 2012... jointly operated

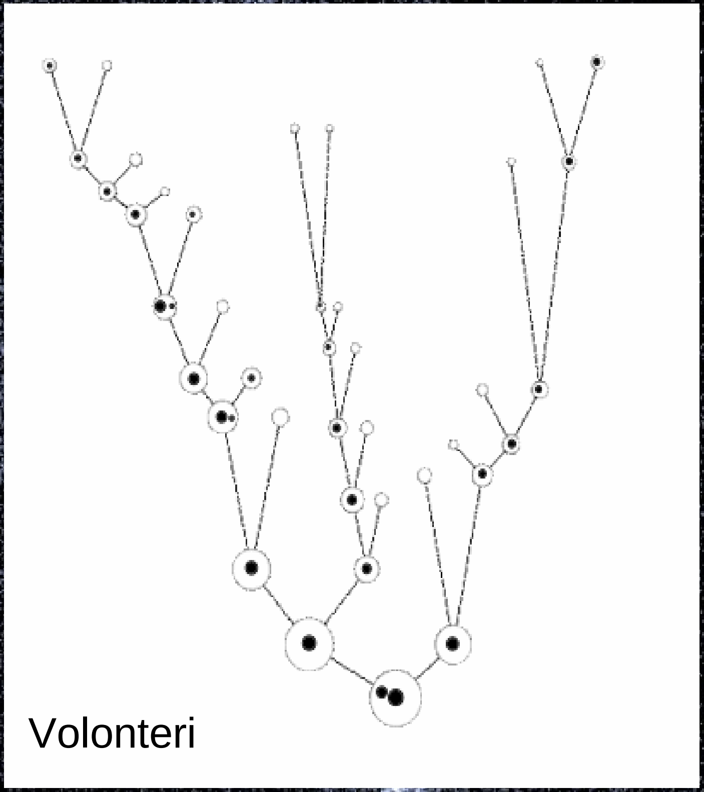


Star Clusters, Black Holes, Gravitational Waves

- Hardware accelerated
- Astrophysics: Black Holes, gravitational waves...
- Software and Scaling

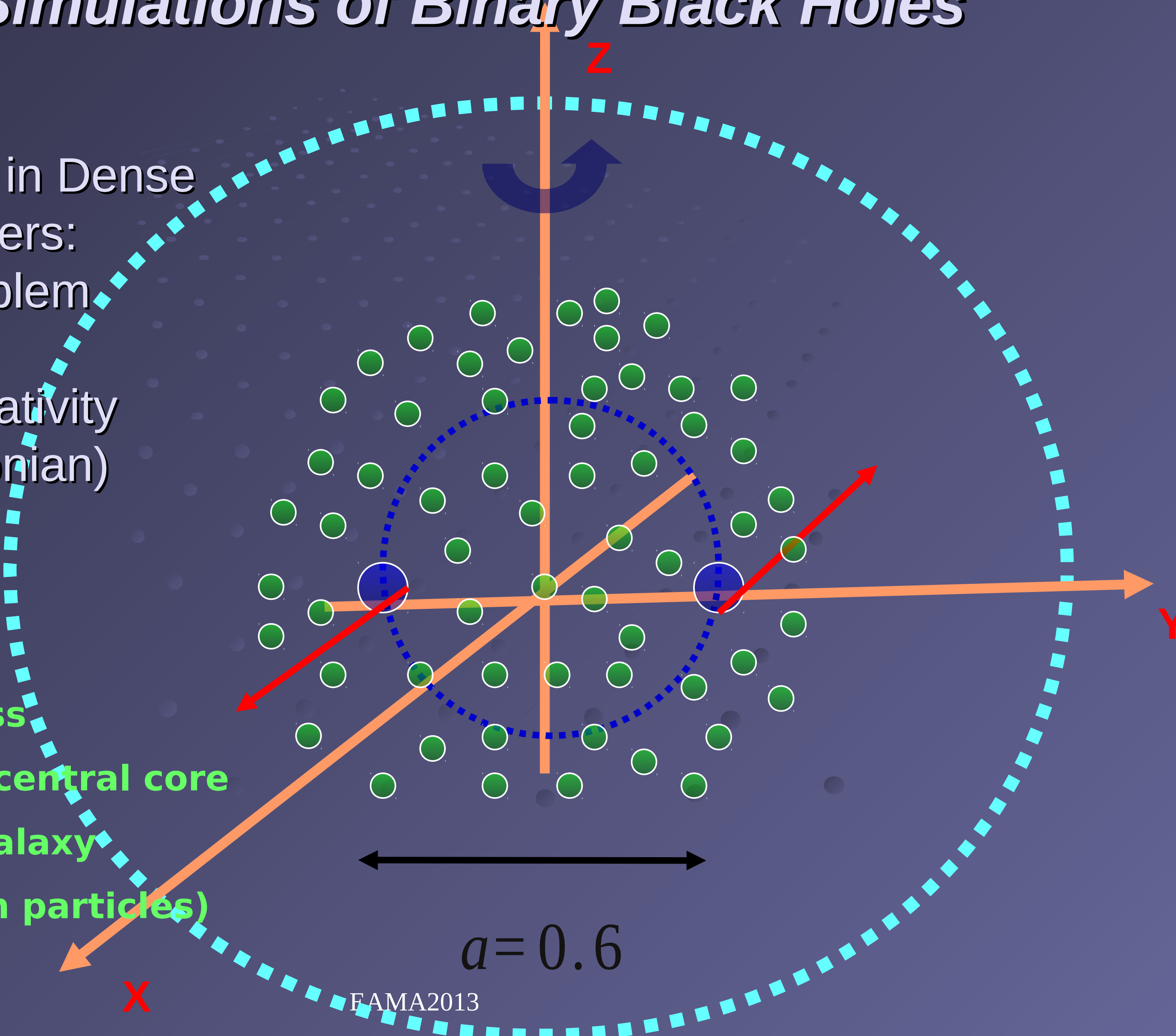
Galaxies merge, hierarchical Structure formation, their centres? Black Holes?





Simulations of Binary Black Holes

Black Holes in Dense
Stellar Clusters:
N-Body Problem
with
General Relativity
(Post-Newtonian)



Two equal-mass
black holes in central core
of simplified galaxy
(up to 4 million particles)

On the Evolution of Stellar Systems

V. A. Ambartsumian

(George Darwin Lecture, delivered on 1960 May 13)

IN THIS lecture we shall consider some aspects of the problem of the evolution of stellar systems. We shall concentrate chiefly on *galaxies*. However, at the same time we shall treat here some questions connected with star *clusters* as component members of galaxies.

Concepts discussed:

Total Energy of grav. star clusters NOT additive

No thermodynamical equilibrium

Statistical Theory of Gases to be used with care (large mean free path)

Locally truncated Maxwellian distribution.

- Millisecond Pulsars — 10^(-3) sec
- Dynamical Time Scale — 10^6 yrs
- Relaxation Time Scale — 10^8 yrs
- Age of Universe — 10^10 yrs

$$t_{\rm cr} = \frac{r_h}{\sigma_h} \,,$$

$$t_{\rm rx} = \frac{9}{16\sqrt{\pi}} \frac{\sigma^3}{G^2 m \rho \ln(\gamma N)} \,.$$

Laboratories for gravothermal N-Body Systems!

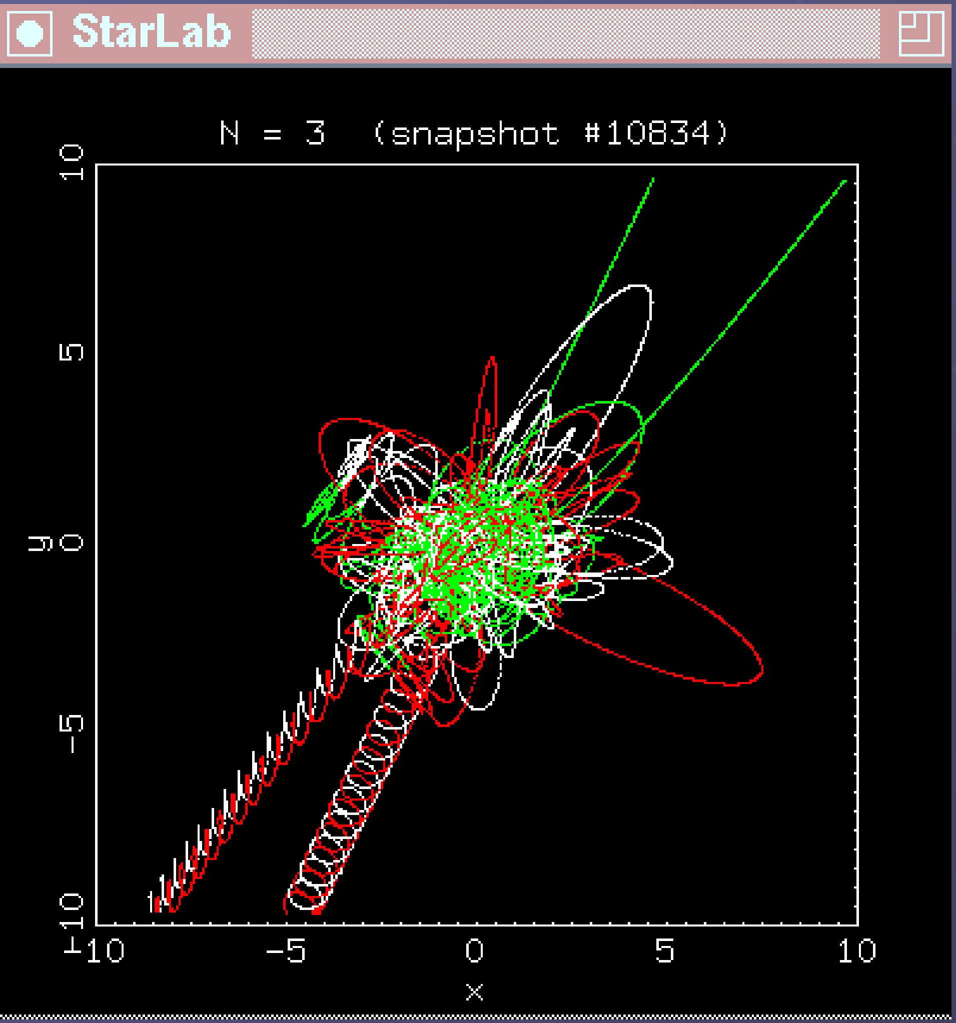
Note: Cosmological and Galactic N-Body Simulations need few crossing times, and less than a relaxation time, while gravothermal systems need multiples of N crossing times, several relaxation times! Complexity goes as N_3 !

$$t_{\rm cr} \approx \sqrt{\frac{r_h^3}{G M_h}} \,.$$

← Virial Equilibrium →

$$\frac{t_{\rm rx}}{t_{\rm dyn}} \propto \frac{N}{\log(\gamma N)} \,.$$

Dynamics of Binary Black Holes in Galactic Nuclei



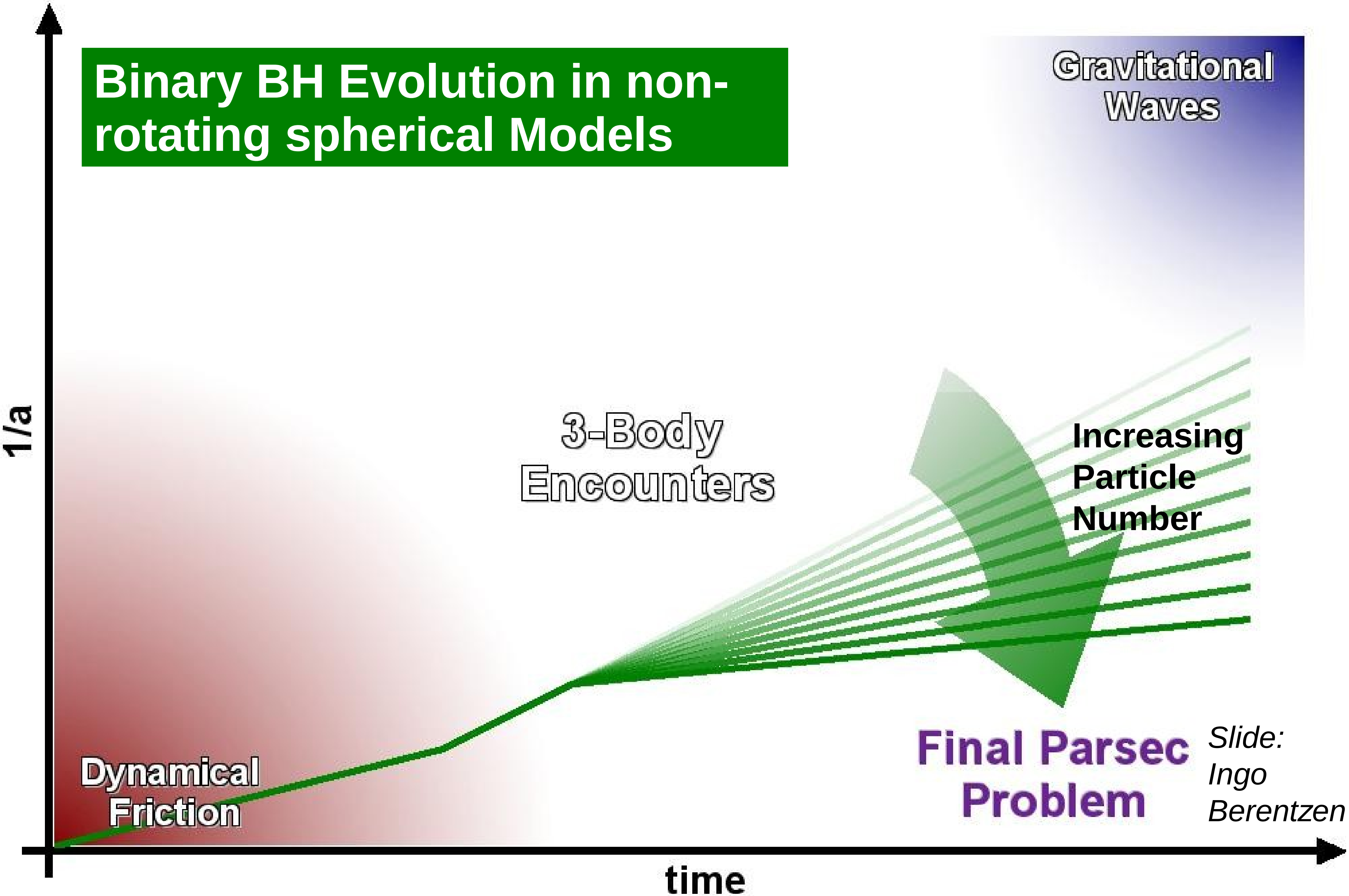
- Unstable 3-body Encounters Starlab Simulation (S.L.W. McMillan)

http://www.physics.drexel.edu/~steve/

-> Three-Body-Problem

Here: some classical 3-body movies...

Binary BH Evolution in non-rotating spherical Models



Slide: Ingo Berentzen

(Khan et al. 2012, ApJ)

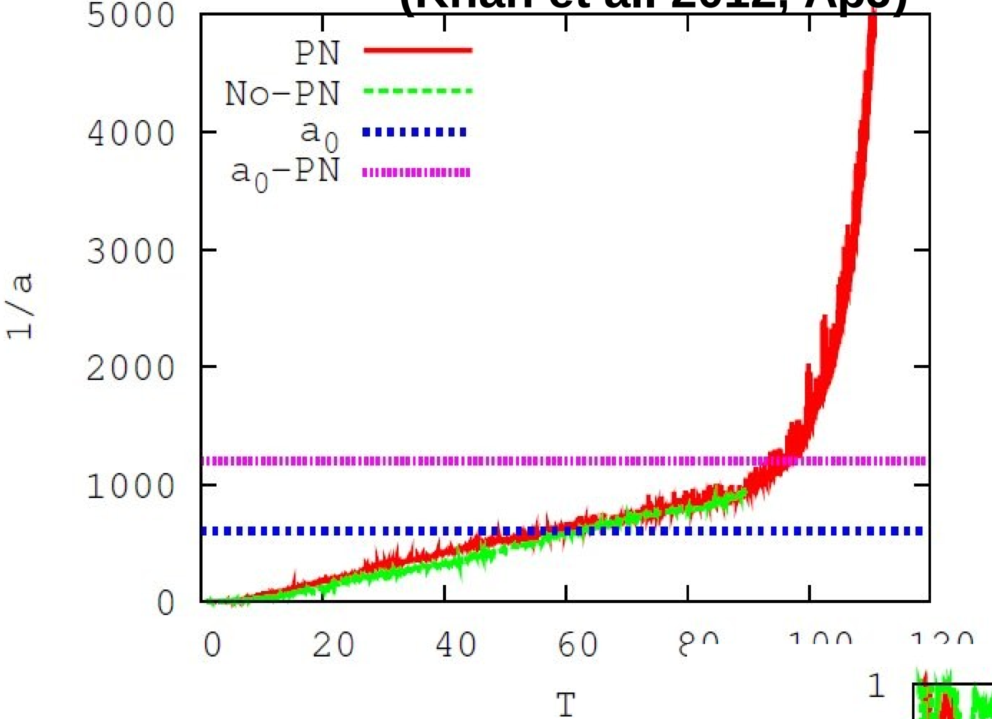
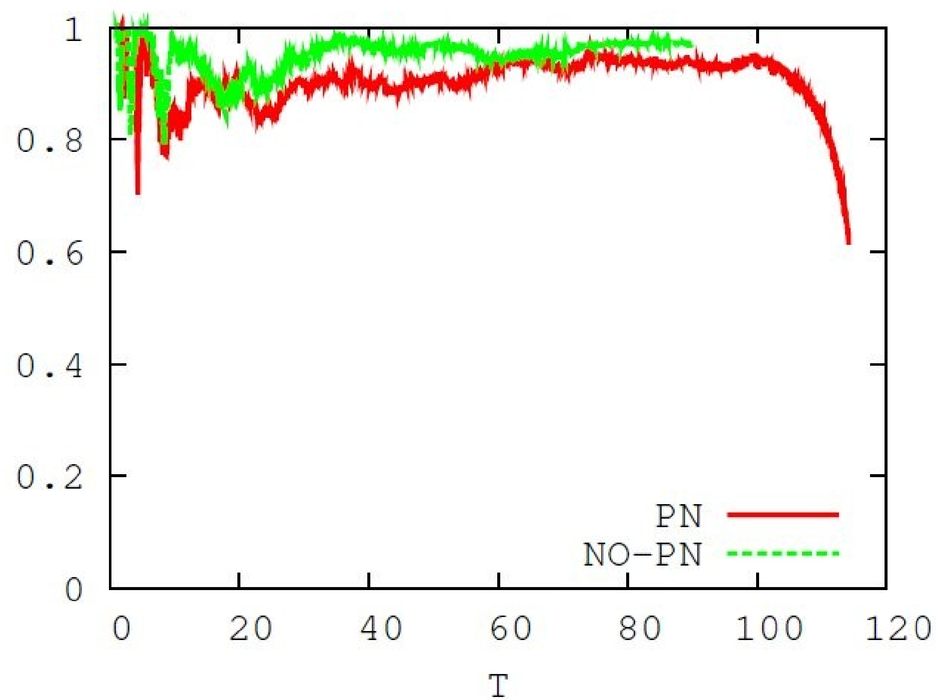


FIG. 7.— Evolution of the inverse semi-major axis $1/a$ (top) and eccentricity e (bottom) for model A2, with and without $\mathcal{PN}$ terms. The horizontal lines represent the estimated semi-major axis of the SMBH binary for which the stellar dynamical hardening becomes equal to the $\mathcal{PN}$ hardening derived from the run without $\mathcal{PN}$ (a_0) and with $\mathcal{PN}$ ($a_0 - \mathcal{PN}$). See main text for further details.

Previous work:

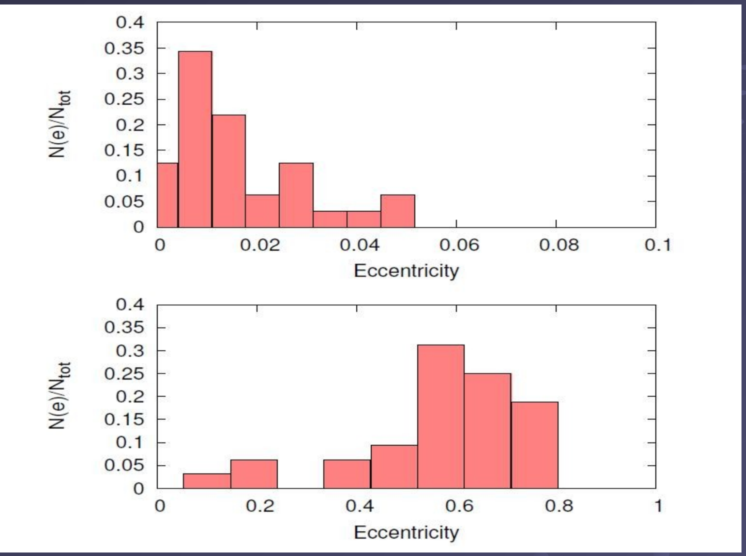
Berczik, Merritt, Spurzem, 2005, ApJ
Berczik, Merritt, Spurzem, Bischof, 2006, ApJ
Berentzen, Preto, Berczik, Merritt, Spurzem, 2009, ApJ
Fiestas & Spurzem, 2010,11 MNRAS
Amaro-Seoane, ..., Sp, MNRAS 2010
Preto, Berentzen, Berczik, Spurzem et al. 2011, ApJ
Khan et al. 2011a, b, ApJ



Time Scale for GR merger: $t_{GR} \propto M^{-3}(1-e^2)^{7/2}$

Important for Background of Ultra-Low GR frequencies (LISA!) 0.01-1 μHz

Dynamics of Supermassive Single and Binary Black Holes in Galactic Nuclei

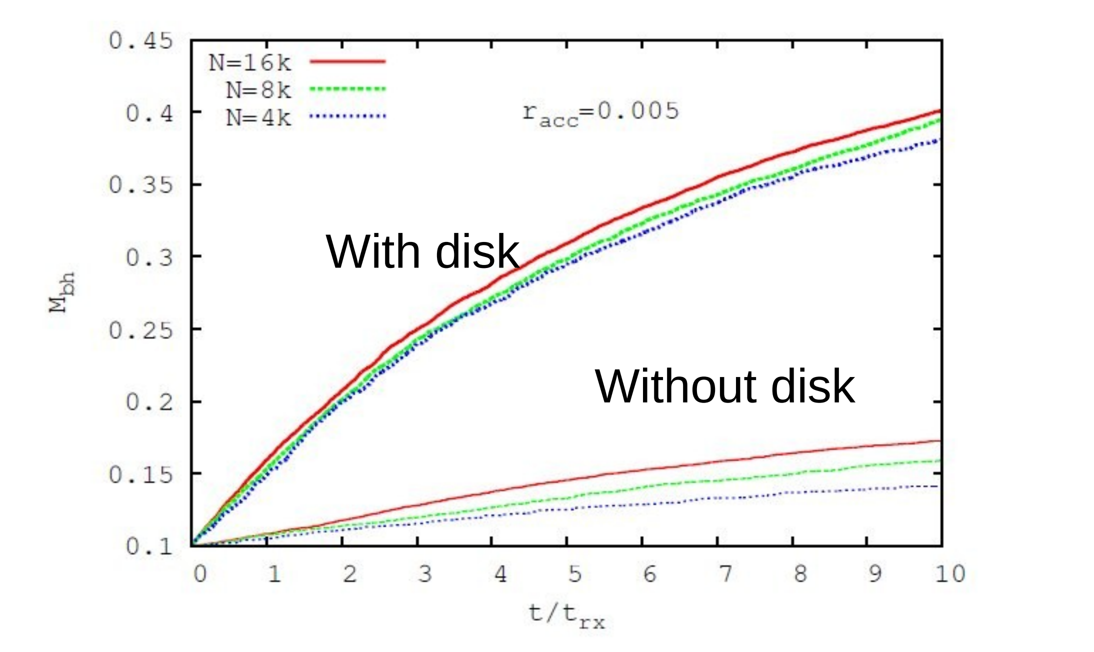


Eccentricity Matters
-
Preto, Berentzen, Berczik, Spurzem, 2011, ApJ
Khan, Berentzen, Berczik, Just, Mayer, Nitadori, Callegari, 2012, ApJ

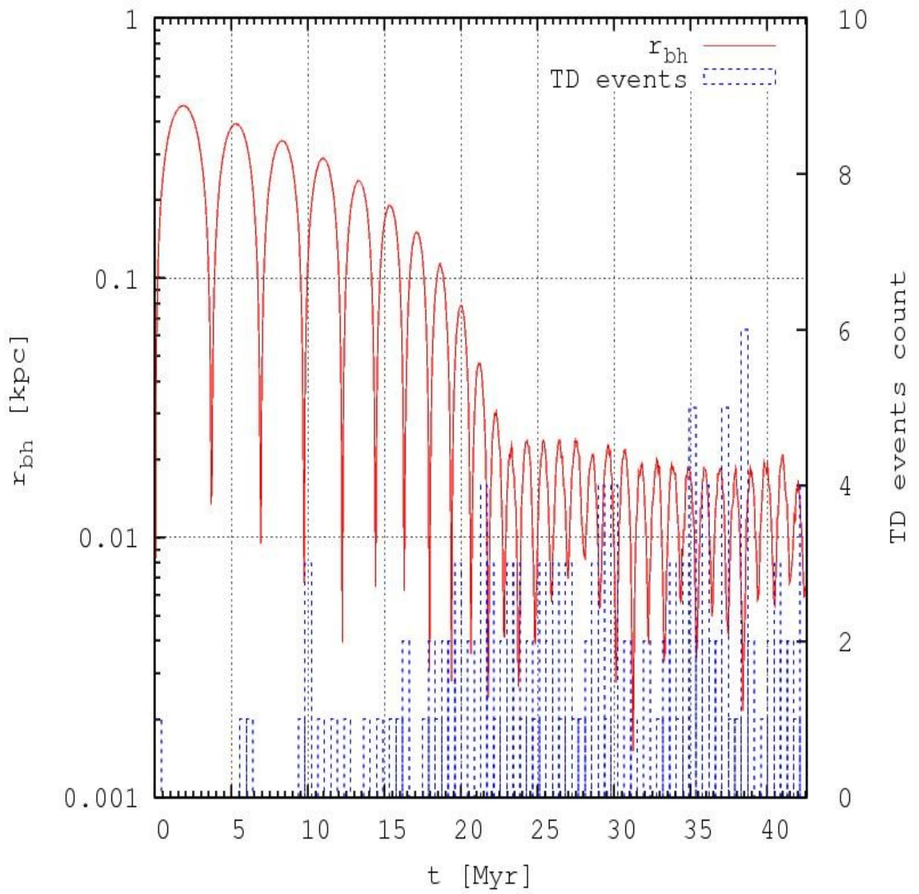
Figure below, from Just, ... Berczik, Spurzem, ..., 2012, ApJ

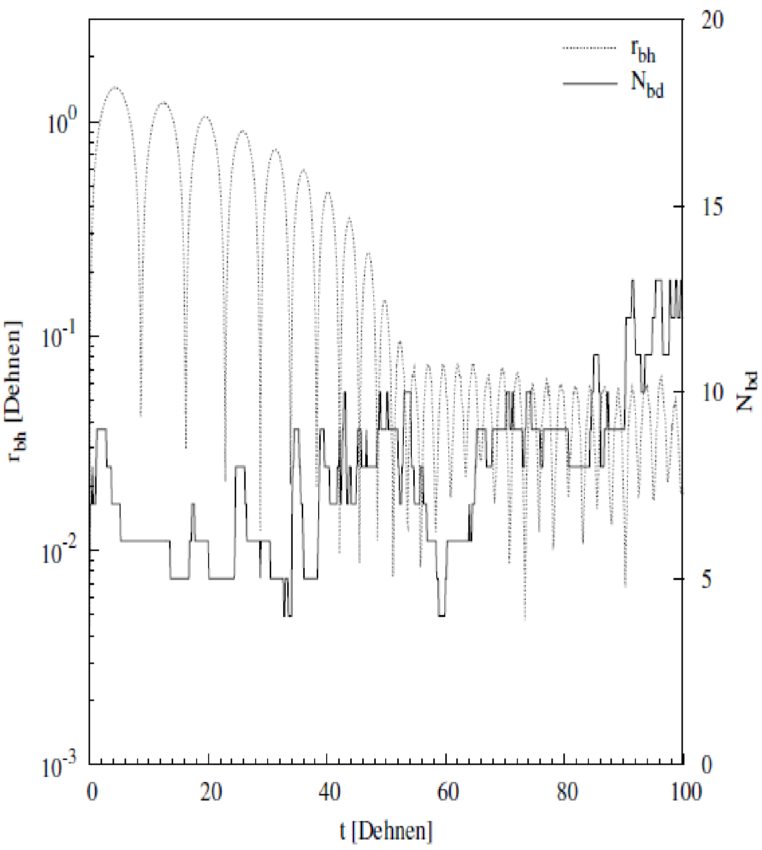
The presence of an accretion disk near an SMBH enhances the mass growth rate of SMBH by factor 3.

Figure on top: lower panel: eccentricity when supermassive binary black hole (SMBH) becomes bound.
Upper panel:
eccentricity shortly before Final relativistic merger. This is important to predict gravitational waveforms correctly.



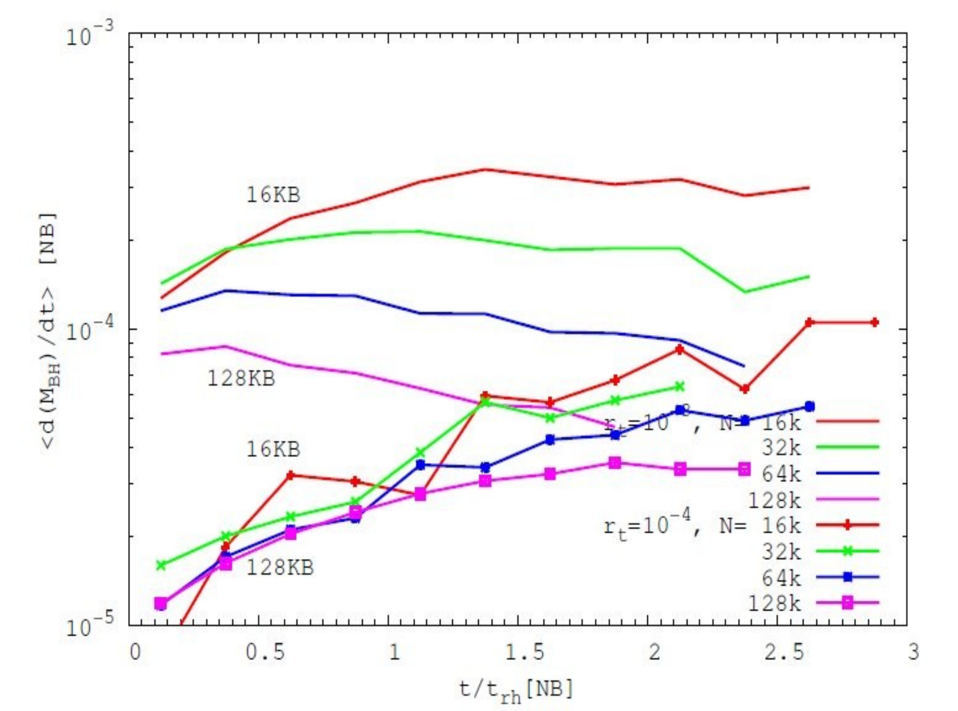
Recoiling Black Hole after GR induced merger in galactic nucleus
Li, Liu, Berczik, Chen, Spurzem, ApJ 748, 65 (2012)





Direct N-Body Simulation (φGPU code), 250k particles; left: Phase 1: black hole oscillates in galactic center (red curve), phase 2: after 20 Myr back in center. Tidal Disruption rate of stars: low in phase 1, surges in phase 2 (blue boxes). TD = tidal disruption – X-ray signature. Right: Ultracompact stellar system around Black hole, oder 10 stars tightly bound.

Black Hole Growth by Tidal Accretion



Zhong, Berczik, Spurzem,
Submitted ApJ 2013

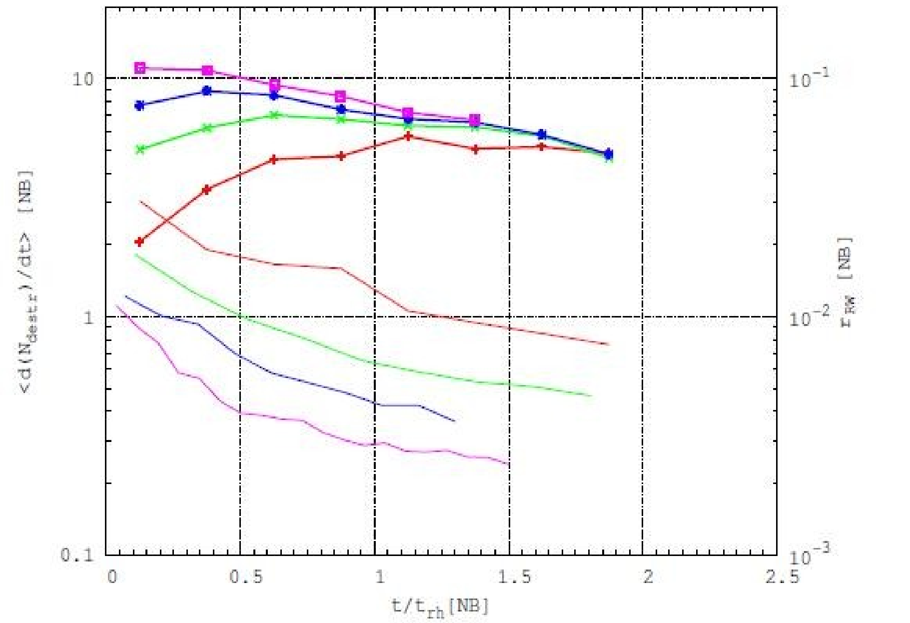


FIG. 2.— x axis is time expressed in unit of initial half-mass relaxation time(t_{rh}), left y axis is the averaged disruption rate in a given time range(i.e. 1/4 t_{rh}). The unit for disruption rate is number of disrupted stars per unit time. Right y axis is the Brownian motion amplitude. Curves with symbols are TD rate for $r_t = 10^{-3}$, from bottom to top, respond for N=16k,32k,64k and 128k. Curves without symbols shows black hole's Brownian motion amplitude for N=16k,32k,64k and 128k(from top to bottom)

Post-Newtonian Dynamics

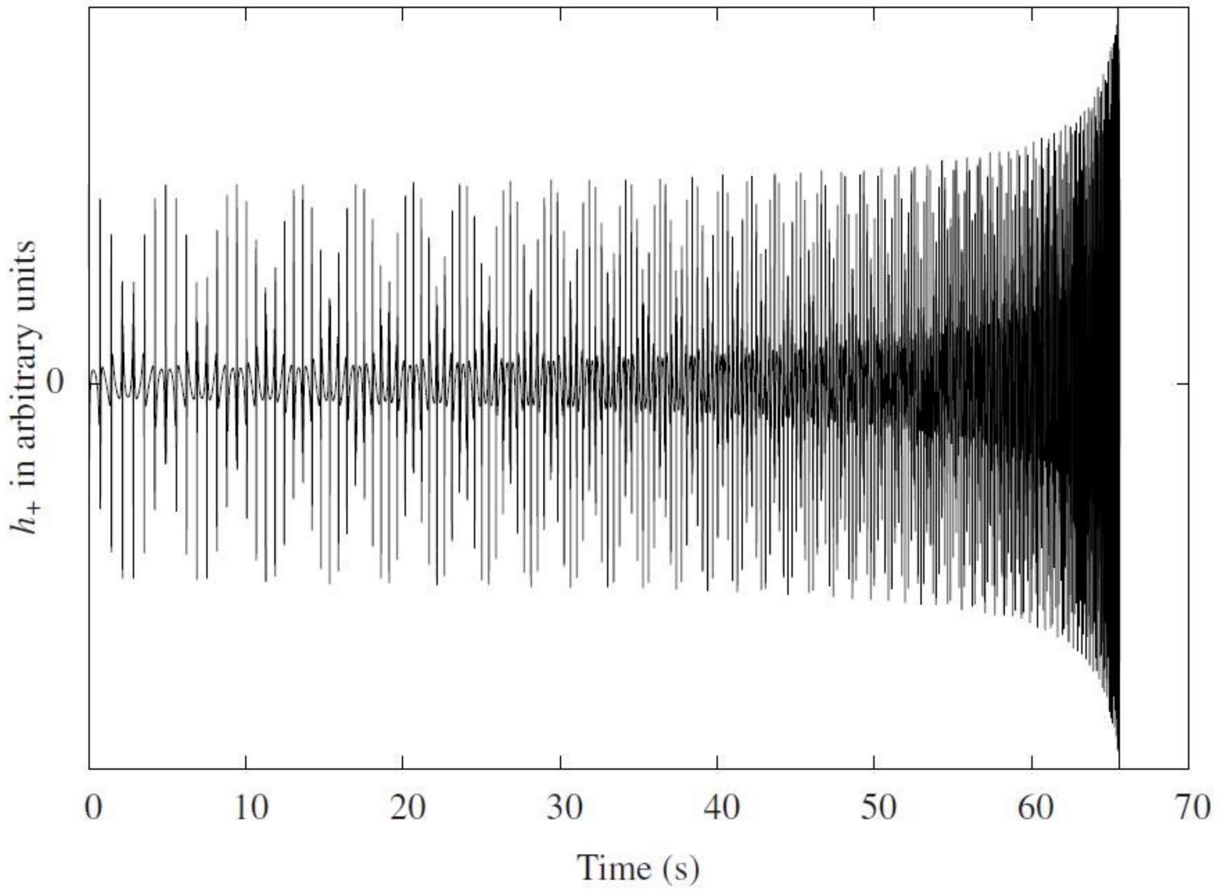


Figure 3.11: Waveform for two equal mass objects on a an orbit with $e = 0.5$.

Plots of h+(t) showing 3 relevant time scales
Orbital evolution is NOT adiabatic (fully 3.5PN accurate)
Handle arbitrary eccentricities (P.Brem, R. Spurzem, Univ. Heidelberg)

Post-Newtonian Dynamics
Gravitational Wave Templates

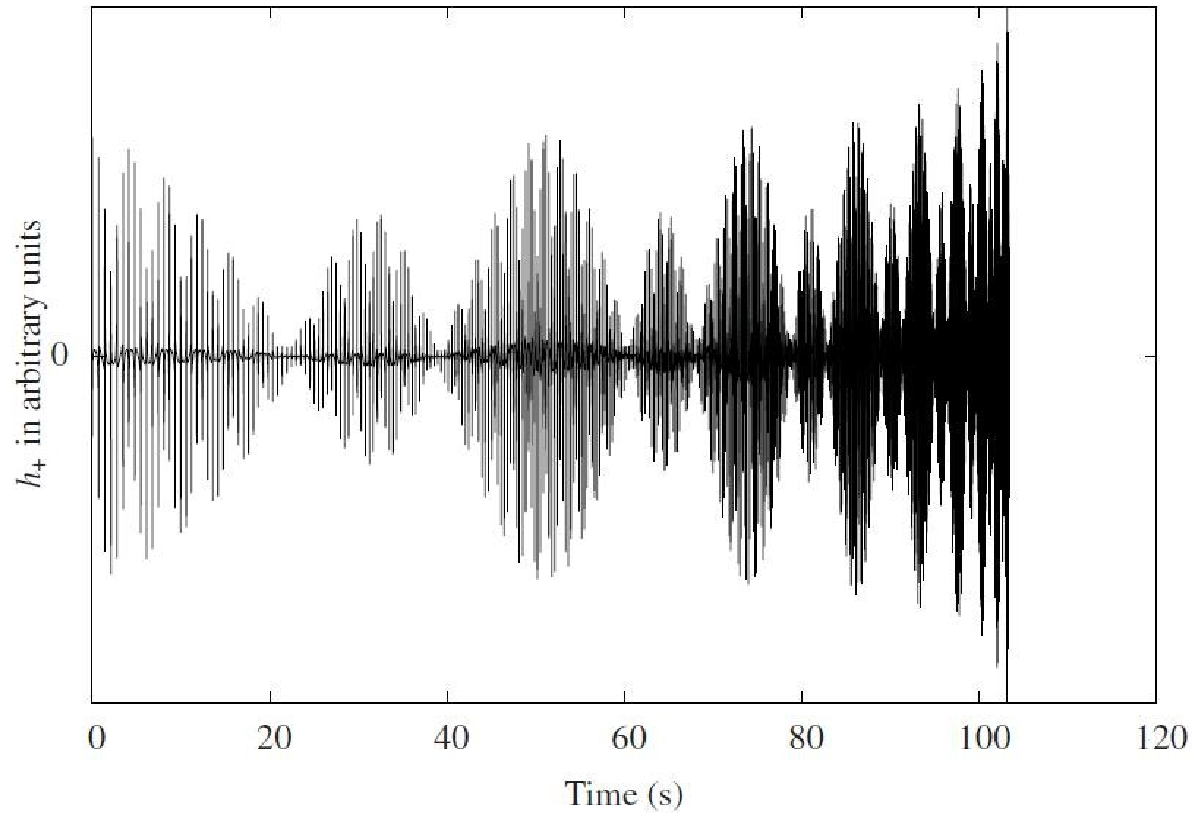
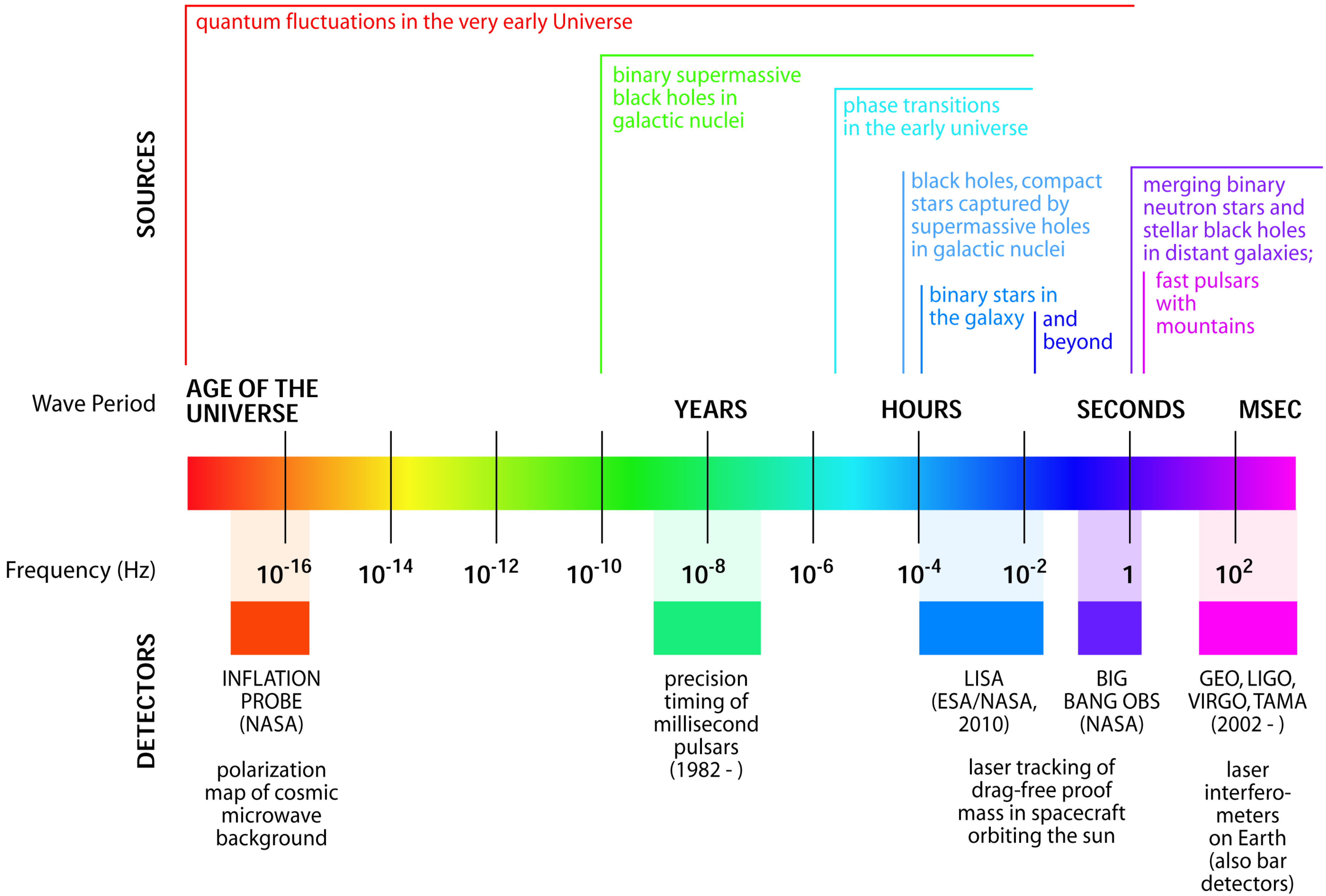


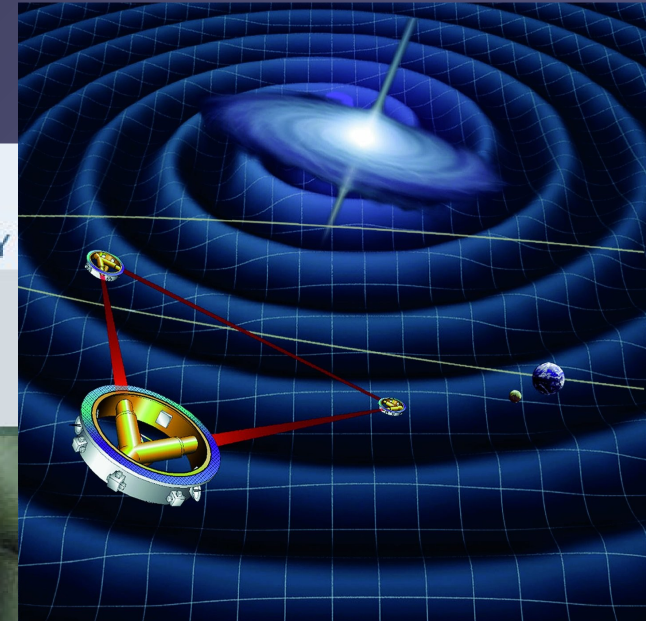
Figure 3.12: Waveform for two objects with a mass ratio of $q = 1/10$ on an orbit with $e = 0.5$ and spins $a_{1,x} = 1.0$, $a_{2,y} = 1.0$.

Handle spin-orbit and spin-spin coupling (P.Brem, R. Spurzem, Univ. Heidelberg)

THE GRAVITATIONAL WAVE SPECTRUM



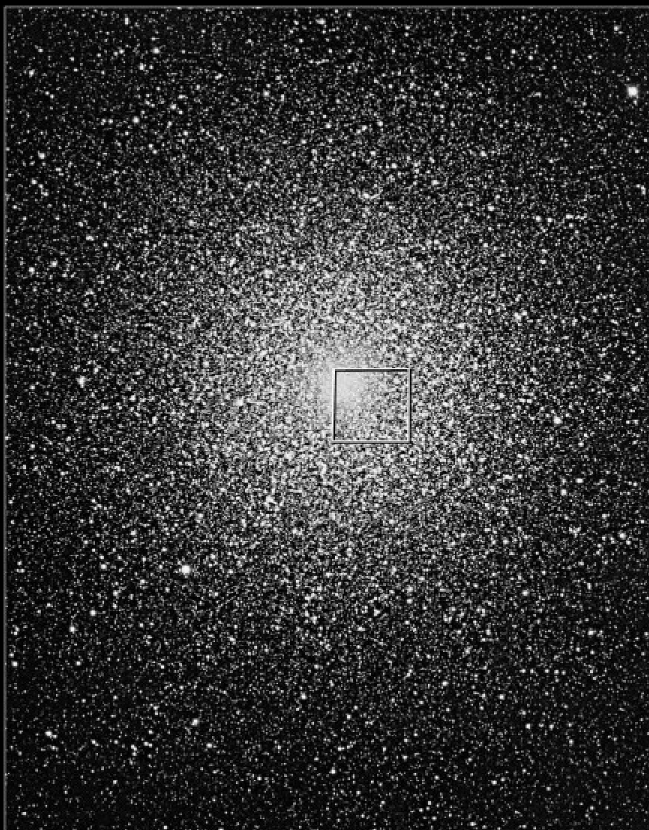
VIRGO Detector in Cascina near Pisa, Italy



LISA =
Laser Space
Interferometer Antenna

$$\vec{a}_0 = \sum_j G m_j \frac{\vec{R}_j}{R_j^3} \quad ; \quad \dot{\vec{a}}_0 = \sum_j G m_j \left[\frac{\vec{V}_j}{R_j^3} - \frac{3(\vec{V}_j \cdot \vec{R}_j)\vec{R}_j}{R_j^5} \right]$$

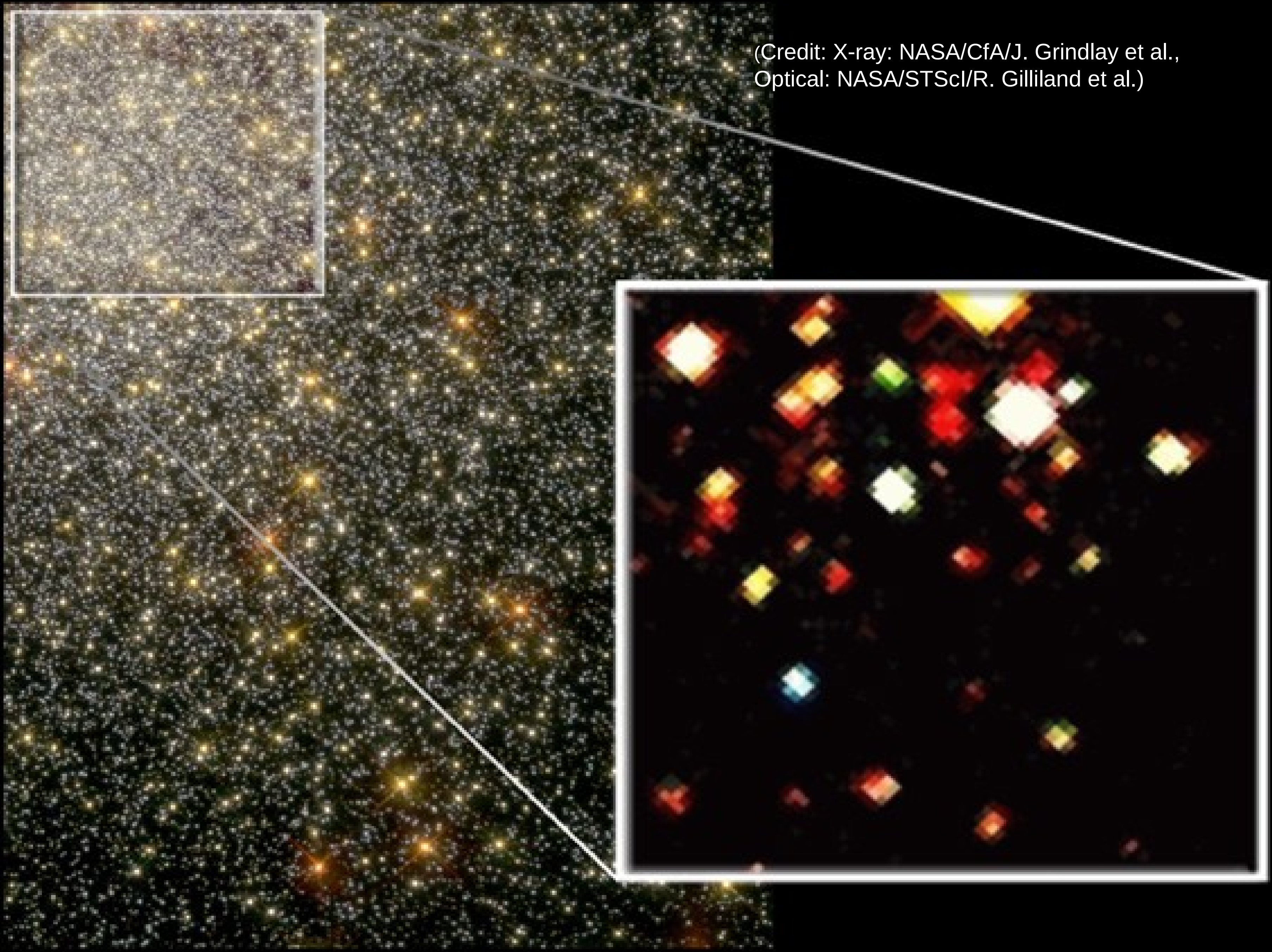
Globular Cluster 47 Tucanae



Ground • AAT

Hubble Space Telescope • WFPC2

NASA and R. Gilliland (STScI)
STScI-PRC00-33



(Credit: X-ray: NASA/CfA/J. Grindlay et al., Optical: NASA/STScI/R. Gilliland et al.)

Compact Binaries in Star Clusters I - Black Hole Binaries Inside Globular Clusters

MNRAS 2010

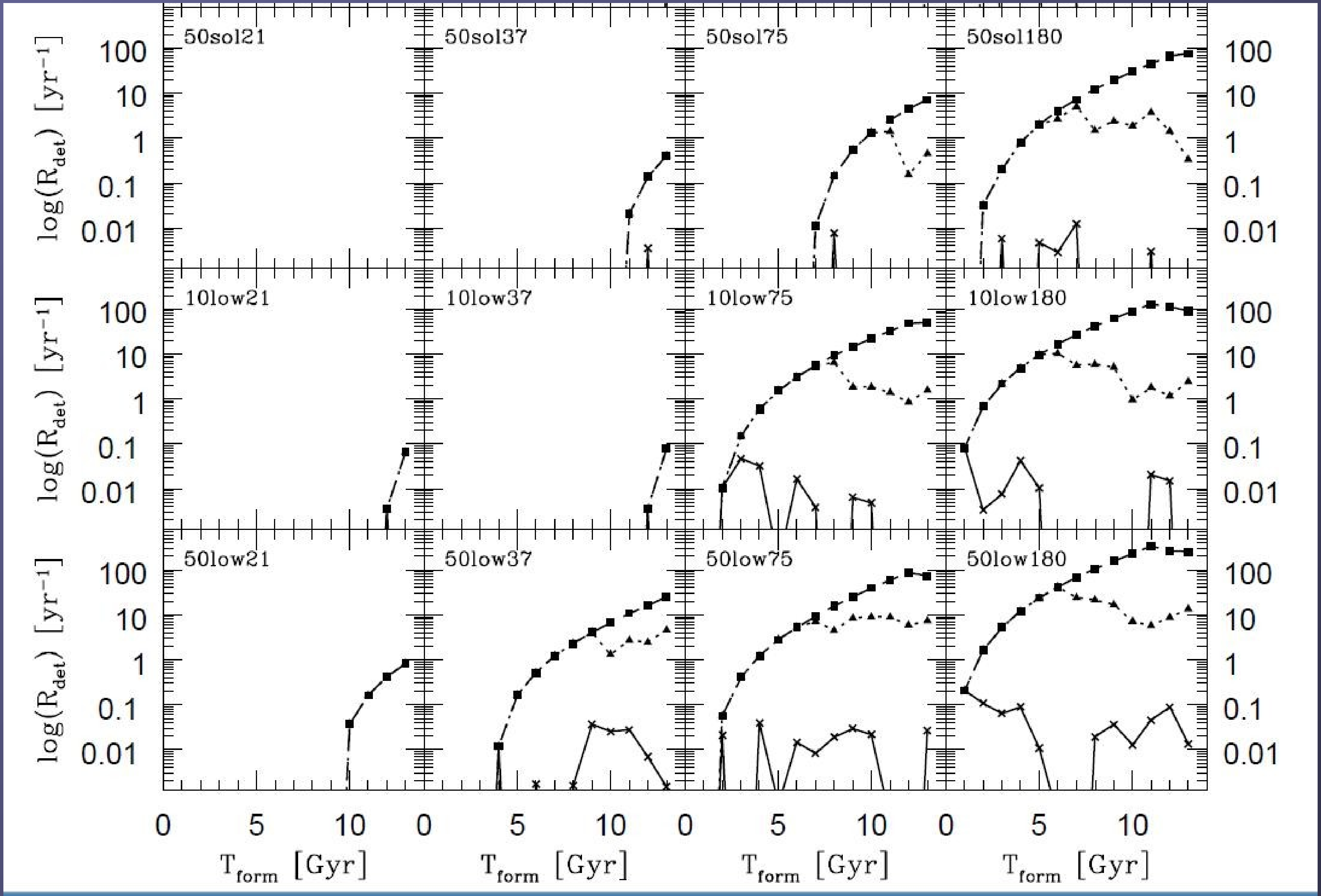
J. M. B. Downing[3⋆], M. Benacquista[4], R. Spurzem[1,2,3], and M. Giersz[5]
[1] National Astronomical Observatories, Chinese Academy of Sciences, 20A Datun Ln, Chaoyang District, 100012, China
[2] Kavli Institute of Astronomy and Astrophysics, Peking University, Beijing, China
[3] Astronomisches Rechen-Institut, Zentrum für Astronomie der Universität Heidelberg, Monchhofsraße 12-14, D-69120 Heidelberg, Germany
[4] Center for Gravitational Wave Astronomy, University of Texas at Brownsville, Brownsville, TX 78520, USA
[5] Nicolaus Copernicus Astronomical Center, Polish Academy of Sciences, ul. Bartycka 18, 00-716 Warsaw, Poland

Compact Binaries in Star Clusters II - Escapers and Detection Rates

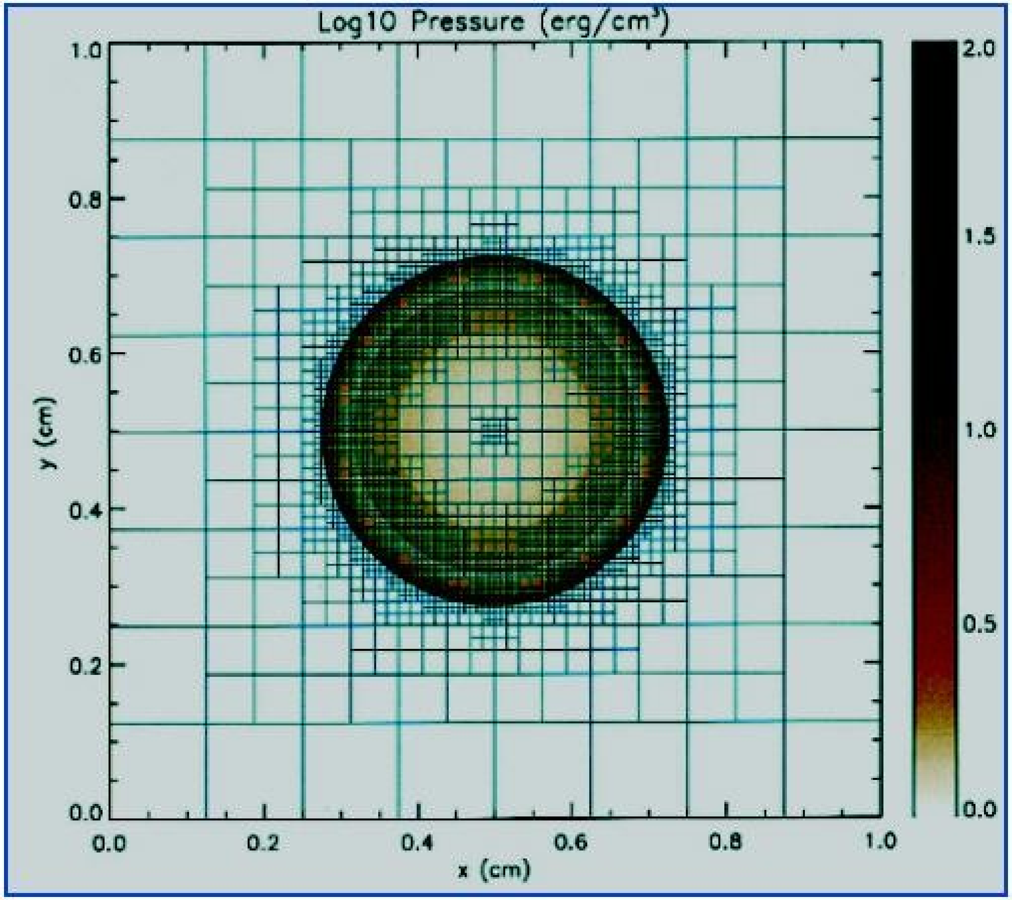
MNRAS 2011

J. M. B. Downing[1,2⋆], M. J. Benacquista[3], M. Giersz[4], and R. Spurzem[5,6,1]
[1] Astronomisches Rechen-Institut, Zentrum für Astronomie der Universität Heidelberg, Monchhofsraße 12-14, D-69120 Heidelberg, Germany
[2] Fellow of the International Max-Planck Research School for Astronomy and Cosmic Physics at the University of Heidelberg, Heidelberg, Germany
[3] Center for Gravitational Wave Astronomy, University of Texas at Brownsville, Brownsville, TX 78520, USA
[4] Nicolaus Copernicus Astronomical Center, Polish Academy of Sciences, ul. Bartycka 18, 00-716 Warsaw, Poland
[5] National Astronomical Observatories, Chinese Academy of Sciences, 20A Datun Rd., Chaoyang District, 100012, China
[6] Kavli Institute of Astronomy and Astrophysics, Peking University, Beijing, China

Downing et al. 2011



Hydrodynamics on a grid



$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla} \cdot \rho \boldsymbol{v} = 0 ,$$

$$\frac{\partial \rho \boldsymbol{v}}{\partial t} + \boldsymbol{\nabla} \cdot \rho \boldsymbol{v}\boldsymbol{v} + \nabla P = \rho \boldsymbol{g} ,$$

$$\frac{\partial \rho E}{\partial t} + \boldsymbol{\nabla} \cdot (\rho E + P)\boldsymbol{v} = \rho \boldsymbol{v} \cdot \boldsymbol{g} ,$$

$$E = \epsilon + \tfrac{1}{2} v^2 ,$$

$$P = (\gamma - 1)\rho\epsilon ,$$

HITS

GAMER – Adaptive Mesh Refinement with many GPU's on Beijing GPU cluster, Schive et al. 2010 (ApJS), Schive, Shukla et al. SC11

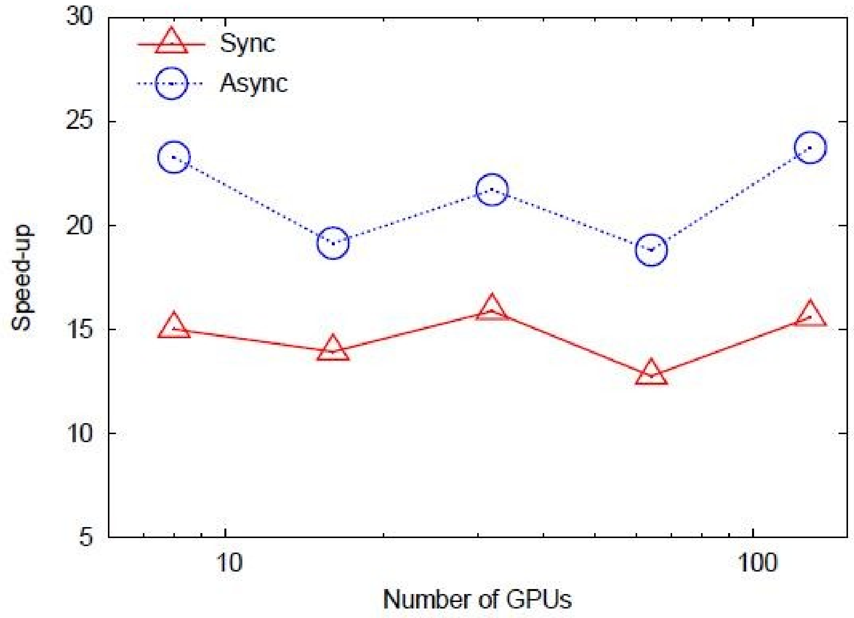


Fig. 1.— Performance speed-up as a function of the number of GPUs/CPUs. For each data point, we compare the performance by using the same number of GPUs and CPU cores. The blue circles and red triangles show the timing results with and without the concurrent execution between CPUs and GPUs, respectively. The speed-up achieved in the 128-GPU run is 23.7x.

Some simulation details:

(1) Root-level resolution	: 256^3
(2) Number of refinement levels	: 7
(3) Highest effective resolution	: $32,768^3$
(4) Total memory consumption	: ~100 GB
(5) Total number of grids	: $\sim 1.8 * 10^9$
(6) Number of GPUs/CPU cores	: 8, 16, 32, 64, 128

Other ongoing projects

Radio Astronomy: Chen Xuelei, Tian Haijun

Galaxy Merger: Yan Yanbin

Shangfei Liu, Doug Lin: Debris Disks around Planets

Gareth Kennedy, et al.: Star-Disk interactions in AGN

Pang Xiaoying, Christoph Olczak, w. GALEV team, Arches cluster

....

Visualization Project with SC-CNIC/CAS

....

See monthly reports of Li Changhua in

http://cic.bao.ac.cn/?page_id=198

...

Interested Users contact: laohu_admin@nao.cas.cn (Chinese/English)

It is Li Changhua, Peter Berczik, Li Shuo, Rainer Spurzem

ICCS Invitation

Founding Members:
NAOC, NACC (Nagasaki)
LBNL, Heidelberg
Contact with KIAS, ...

http://iccs.lbl.gov

Building International Community

Invitation to join at different level:

- (I) Provide hardware access and support for green network of GPU clusters (currently Berkeley dirac, Heidelberg titan, Beijing laohu, Nagasaki dejima invited)
- (II) Take part in individual collaborations, community building by bridging the disciplines, contribute to database of benchmarks and tools, workshops, publications

* (III) Take part in Technical Working Groups

Education and Outreach

Invitation to 3rd ICCS School and Workshop

Stanford 2010, Berkeley 2011, Beijing, NAOC, 2012
next workshop to be decided spring 2014 (Germany, Japan, Korea, US?)

NAOC 中国科学院国家天文台 NATIONAL ASTRONOMICAL OBSERVATORIES ,CHINESE ACADEMY OF SCIENCES

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Summary

- **Astrophysical High Precision N-Body -**
  Ready for million core and Exascale (also other apps.)

- **Community forms along extended Silk Road**
  Physics/Astrophysics/Accelerators ICCS
  Schools and Workshops (Stanford 2010, Berkeley 2011, Beijing 2012, ...) http://iccs.lbl.gov
  Technical Working Groups (-> need more life)
  Benchmarks (-> better than top500?)

- **Astrophysical Science Drivers:**
  Gravitational Waves from Distant Black Holes
  Is Einstein right? Do spinning black holes exist?
  Electromagnetic radiation follow-up to GW?
  Current resolution (million bodies) not enough...
  Basic Science...