

**GPU Supercomputing** 



**Uni Heidelberg** 

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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?



Support and Collaboration by CNIC @ NAOC (Chenzhou CUI and team)

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



The Kavli Institute for Astronomy and Astrophysics at Peking University 北京大学科维理天文与天体物理研究所





#### http://silkroad.bao.ac.cn

National Astron. Observatory of Chinese Academy of Sciences, Beijing China Kavli Institute for Astronomy and Astrophysics, Peking University, Beijing, China Fesenkov Astrophysical Institute, Space Institute, Almaty, Kazakhstan *Institute of Space Technology, Islamabad, Pakistan (NEW)* Main Astronomical Observatory of Ukrainian Academy of Sciences, Kiev, Ukraine Astrophysical Institute Univ. of Vienna, Austria Astronomisches Rechen-Institut,Zentrum f. Astronomie (ZAH) and Computer Engineering and Architecture (ZITI), Univ. Of Heidelberg, Germany Max-Planck Institute for Astrophysics (MPA), Garching/Munich, Germany Instruments (Hardware/Software)
 Dragon Simulations of Star Clusters
 Black Holes / Gravitational Waves

## **GPU Computing**

## NVIDIA TESLA

## PCI Express 2.0

#### GPU

- Number of processor cores: 240
- Processor core clock: 1.296 GHz
- Voltage: 1.1875 V
- Package size: 45.0 mm × 45.0 mm 2236-pin flip-chip ball grid array (FCBGA)

**DVIDIA** 

TESLA

#### Board

- Fourteen layer printed circuit board (PCB)
- PCI Express 2.0 ×16 system interface
- Physical dimensions: 4.376 inches × 10.50 inches, dual slot
- Board power dissipation: 187.8 W

#### **External Connectors**

None

Internal Connectors and Headers

- One 6-pin PCI Express power connector
- One 8-pin PCI Express power connector
- 4-pin fan connector

## General Purpose General Purpose GPGPU Supercomputing (GPGPU)

http://www.nvidia.com
http://www.astrogpu.org

#### http://gpgpu.org

#### NVIDIA Tesla C1060 in kolob cluster Heidelberg Univ.









#### Our Green Grid: GPU Clusters used:

老虎 Beijing <u>(NAOC/CAS and Silk Road Project)</u> 85 Nodes, 64 Kepler K2

Max-Planck MPCDF GPU cluster (400 Kepler K20 GPUs) Golowood cluster, Main Astron. Observatory, Kiev, Ukraine Kepler cluster Heidelberg, Germany (12x Kepler GPU)





## NAOC laohu cluster 64 Kepler K20



Request: New and/or upgrade of laohu

Laohu: 2009/2013 (Kepler GPU) 100 Tflop/s 150k cores

Need for GW research: ~100 Pascal GPU 1.5 Pflop/s 300k cores

Compare: AEI Hannover B. Allen

**MPG Garching Hydra** 

#### Kepler Scaling, it works...



Spurzem, Berczik, et al., 2013, LNCS Supercomputi 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.

#### **Pascal Scaling, it works...**



Pascal GF1080 TITAN (Kepler) Kepler K20m Spurzem, Berczik, et al., 2013, LNCS Supercomp

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. X = first GPU of laohu 2010

## Nr. 1,2 Supercomputer from China: 96/33 Pflop/s Linpac Wuxi/Guangzhou/Tianjin National Supercomputing Cen Taihu 10 mill. cores

Tianhe-2 (MilkyWay-2) - TH-IVI E5-2692 12C 2.200GHz, TH Ex 31S1P



Test of Taihu planned; But: Local cluster with new GPUs at NAOC gives much more

## Intel MIC Hardware INSPUR, NAOC - 2013.XI.26



icpc ... "-mmic" ... 61 x 4 = 244 x 1.1 GHz omp cores !!! Full fp64 !!!



PEKING UNIVERSITY

NATIONAL ASTRONOMICAL OBSERVATORIES , CHINESE ACADEMY OF SCIENCES

#### Software

NBODY4, NBODY6, S.J.Aarseth, S. Mikkola, ... (ca. 20.000 lines, since 1963):

- Hierarchical Individual Time Steps (HITS)
- Ahmad-Cohen Neighbour Scheme (ACS)
- Kustaanheimo-Stiefel and Chain-Regular. (KSREG) for bound subsystems of N<6 (Quaternions!)</li>
- 4th order Hermite scheme (pred/corr), Bulirsch-Stoer (for Chain)
- Stellar Evolution (single/binary) (w Hurley)

#### •<u>NBODY6++GPU, φGPU, L. Wang, R. Spurzem, P. Berczik, K.</u> <u>Nitadori,...</u>

- (massively parallel codes, since 1999, recent paper Wang, Spurzem, Aarseth, et al. 2015):
- NBODY6++ (Spurzem 1999) using MPI
- Parallel φGRAPE / φGPU (Harfst et al. 2006, Spurzem et al. 2009)
   NBODY6++/GPU-MPI (Wang, Spurzem, Aarseth, et al. 2015)
- Parallel Binary Integration in Progress (KSREG)

## Our CPU/GPU N-body (AC) code NBODY6++GPU Wang, Spurzem, Aarseth, et al. 2015, 2016 → Exaflop/s Huang, Berczik, Spurzem 2016 **Typical: 8/16 GPUs** → **19000/38000 cores** GPU GPU GPU Node 5 GPU GPU GPU Node

https://github.com/lwang-astro/betanb6pp

Node ...

## NBODY6++ PERFORMANCE OF HYBRID MPI







Fig. 2 The speed-up (S) of NBODY6++ as a function of particle number (N) and processor number  $(N_p)$ . Solid points are the measured speed-up ratio between sequential and parallel wallclock time, dash lines predict the performance of larger scale simulations further. The symbols used in figure have the magnitudes:  $1k = 1,024, 1M = 1k^2$  and  $1G = 1k^3$ .

Huang, Berczik, Spurzem, RAA, 2015



Fig. 5 The speed-up (S) of Bonsai as a function of particle number (N) and processor number  $(N_p)$ . Solid points are the measured speed-up ratio between sequential and parallel wall-clock time, dash lines predict the performance of larger scale simulations further. The symbols used in figure have the magnitudes:  $1k = 1,024, 1M = 1k^2$  and  $1G = 1k^3$ .

## "Moore's" Law for Direct N-Body



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# Instruments (Hardware/Software) <u>Dragon Simulations of Star Clusters</u> Black Holes / Gravitational Waves

## On the Evolution of Stellar Systems

#### V. A. Ambartsumian

(George Darwin Lecture, delivered on 1960 May 13)

N 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.







Ground • AAT

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

Hubble Space Telescope • WFPC2



## Approx. Models: Fluid Dynamics/Fokker-Planck



Bettwieser & Sugimoto 1984: Gravothermal Oscillations by energy generation from binaries (cf. nuclear stellar energy generation MODEST-16

Cohn (1980): Direct Fokker-Planckj mode Core Collapse Gravothermal Catastrophe



Figure 1. The 'central' density  $\psi_c$  is plotted against the non-dimensional time  $t/t_{ref}$  for k = 2 models with three different values of C as attached to each curve. Note, that if they were plotted with the same ordinate they would be close to each other despite the great differences in C. The model indicated with a filed circle will be compared with King's model in Section 4.2.

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

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

-> Three-Body-Problem



Gravothermal Oscillations -Attractor in Phase Space Spurzem 1994, Giersz & Spurzem 1994 Amaro-Seoane, Freitag & Sp. 2004



Fig. 3: Projected three-dimensional attractor for N = 100.000 system,  $x = \log \rho'_c$ ,  $y = \log \sigma'_c$ ,  $z = \xi$ .

Follow-Up of Angeletti & Giannone and Larson CAS 2016 武汉

### **Theoretical Models II: Fokker-Planck**

#### **Dissolution of Star Cluster in Tidal Field**



Kim, Yoon, Lee, Spurzem, 2008, MNRAS

Hong, Kim, Lee, Spurzem, 2013, MNRAS

Three Phases in Cluster Dissolution: 1) Core Collapse (Encounters) 2) Post-Collapse Steady Evaporation (Encount) 3) Dynamic final dissolution Leiden

## Key Question 1. When will we see the first star-by-star *N*-body model of a globular cluster?

Bottle of Whisky for Million Body Simulation

- Honest N-body simulation
- Reasonable mass at 12 Gyr ( $\sim$ 5x10<sup>4</sup>M<sub> $\odot$ </sub>)
- Reasonable tide (circular galactic orbit will do)
- Reasonable IMF (e.g. Kroupa)
- Reasonable binary fraction (a few percent)
- Any initial model you like (Plummer will do)
- A submitted paper (astro-ph will do)

An inducement: a bottle of single malt Scotch whisky worth €50

#### Awarded to Long Wang MODEST15s Kobe See his talk tomorrow

There are low-mass outlying clusters which have lost little mass. They do not count.

## CPU/GPU N-body6++



Key Question 1. When will we see the first star-by-star *N*-body model of a globular cluster?

· Honest N-body simulation

Leiden

- Reasonable mass at 12 Gyr (~5x10<sup>4</sup>M<sub>o</sub>)
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http://silkroad.bao.ac.cn/dragon/

One million stars direct simulation,

biggest and most realistic direct N-Body simulation of globular star clusters. With stellar mass function, single and binary stellar evolution, regularization of close encounters, tidal field (NBODY6+ +GPU).

(NAOC/Silk Road/MPA collaboration). Wang, Spurzem, Aarseth, Naab et al. MNRAS, 2015 Wang, Spurzem, Aarseth Naab, et al. re-subm. MNRAS 2016



#### 天龙星团模拟:百万数量级恒星、黑洞和引力波 **Dragon Star Cluster Simulations:** MS 20.7M HG Millions of Stars; black holes and RG gravitational waves CHB AGB 15 WD 12 Time = 12 Gyr 20 > 14 16 25 18 0 Gyr 30 0.1 Gyr 1 Gyr 4 Gyr 20

12 Gyr

2.0

1.5

1.0

B-V

0.5

0.0

35

0.0

0.5

1.0

1.5

B-V

2.5

2.0

3.0

#### **Example: DRAGON vs. Observation of NGC4372...**

- + + 0 Myr
- × × 100 Myr

● ● 12000 Myr

🚹 🚹 Obs.

\* \* 1000 Myr

4000 Myr

Kacharev et al. 14



#### **GalevNB: a conversion from N-BODY simulations to observations**

Xiaoying Pang<sup>1,2,5</sup>, Christoph Olczak<sup>1,3</sup>, Difeng Guo<sup>1,3</sup>, Rainer Spurzem<sup>1,4,3,6</sup> and Ralf Kotulla<sup>7</sup>



#### Individual Time Step Storage Scheme for Astrophysical *N*-body Simulations and its Applications <u>ApJS 2015</u>

Maxwell Xu Cai (蔡栩)<sup>1,2</sup>, Yohai Meiron<sup>2,1</sup>, M.B.N. Kouwenhoven<sup>2</sup>,



#### <u>Stardisk Project – Beijing – Almaty – Kiev - Heidelberg</u>

Just, ... Berczik, Spurzem, et a, 2012, ApJ (Paper I) Kennedy, Meiron et al. 2016 MNRAS (Paper II) Panamarev, Shukirgaliev et al. 2017 in prep. (Paper III)

The presence of a gaseous accretion disk near an SMBH enhances the mass growth rate of SMBH and forms a compact stellar disk.



## Instruments (Hardware/Software) Dragon Simulations of Star Clusters <u>Black Holes / Gravitational Waves</u>

## **Post-Newtonian Dynamics**

Method A: use geodetic equations, harmonic gauge, directly obtain eqs. of motion (Blanchet et al.) Method B: Hamiltonian approach using ADM gauge (Schaefer et al.)

A and B equivalent till PN2.5 (1/c\*\*5), higher order gauge functions appear.

$$\frac{dv^{i}}{dt} = -\frac{Gm}{r^{2}}\left[\left(1+\mathcal{A}\right)n^{i}+\mathcal{B}v^{i}\right] + \mathcal{O}\left(\frac{1}{c^{8}}\right),\tag{181}$$

and find [43] that the coefficients  $\mathcal{A}$  and  $\mathcal{B}$  are

$$\begin{split} \mathcal{A} &= \frac{1}{c^2} \left\{ -\frac{3\dot{r}^2\nu}{2} + v^2 + 3\nu v^2 - \frac{Gm}{r} (4+2\nu) \right\} & \text{Perihel shift} \\ &+ \frac{1}{c^4} \left\{ \frac{15\dot{r}^4\nu}{8} - \frac{45\dot{r}^4\nu^2}{8} - \frac{9\dot{r}^2\nu v^2}{2} + 6\dot{r}^2\nu^2 v^2 + 3\nu v^4 - 4\nu^2 v^4 & \dots \text{ higher order...} \\ &+ \frac{Gm}{r} \left( -2\dot{r}^2 - 25\dot{r}^2\nu - 2\dot{r}^2\nu^2 - \frac{13\nu v^2}{2} + 2\nu^2 v^2 \right) + \frac{G^2m^2}{r^2} \left(9 + \frac{87\nu}{4}\right) \right\} \\ &+ \frac{1}{c^5} \left\{ -\frac{24\dot{r}\nu v^2}{5} \frac{Gm}{r} - \frac{136\dot{r}\nu}{15} \frac{G^2m^2}{r^2} \right\} & \text{Grav. Radiation} \end{split}$$

CAS 2016 武汉

## **Post-Newtonian Dynamics**

Indirect Proof by Hulse and Taylor, binary pulsar (Nobel prize 1993)



CAS 2016 武汉

Post-Newtonian Dynamics Spin-Orbit Interaction S / Spin-Spin SS

$$\frac{d\mathbf{v}_{1}}{dt} = \mathbf{A}_{N} + \frac{1}{c^{2}}\mathbf{A}_{1PN} + \frac{1}{c^{3}}\mathbf{A}_{1.5PN} + \frac{1}{c^{4}}[\mathbf{A}_{2PN} + \mathbf{A}_{2PN}] + \frac{1}{c^{5}}[\mathbf{A}_{2.5PN} + \mathbf{A}_{2.5PN}] + \mathcal{O}\left(\frac{1}{c^{6}}\right).$$
(5.1)

Faye, Blanchet, Buonanno 2006

$$\begin{split} \mathbf{A}_{\text{S}1.5PN} &= \frac{Gm_2}{r_{12}^3} \left\{ \left[ 6 \frac{(S_1, n_{12}, v_{12})}{m_1} + 6 \frac{(S_2, n_{12}, v_{12})}{m_2} \right] \mathbf{n}_{12} \\ &+ 3(n_{12}v_{12}) \frac{\mathbf{n}_{12} \times \mathbf{S}_1}{m_1} + 6(n_{12}v_{12}) \frac{\mathbf{n}_{12} \times \mathbf{S}_2}{m_2} \\ &- 3 \frac{\mathbf{v}_{12} \times \mathbf{S}_1}{m_1} - 4 \frac{\mathbf{v}_{12} \times \mathbf{S}_2}{m_2} \right\}. \end{split}$$
(5.3a)

## **Post-Newtonian Dynamics**

Brem, Amaro-Seoane Spurzem, MNRAS 2013

Include Spin-Orbit Spin-Spin PN3, PN3.5 Spin Dynamics

By Patrick Brem (Diploma Thesis Univ. Heidelberg)

1PN 2PN + 1.5PN SO 3PN + 2.5PN SO 2.5PN + 2PN SS 3.5PN



CAS 2016 武汉

#### Rezzolla Final Spin Formula

Brem, Amaro-SeoaneS, Spurzem, MNRAS 2013

$$\begin{aligned} |\mathbf{a}_{\text{fin}}| = & \frac{1}{(1+q)^2} \left[ |\mathbf{a}_1|^2 + |\mathbf{a}_2|^2 q^4 + 2|\mathbf{a}_2| |\mathbf{a}_1| q^2 \cos \alpha \right. \\ & + 2(|\mathbf{a}_1| \cos \beta + |\mathbf{a}_2| q^2 \cos \gamma) |\mathbf{l}| q + |\mathbf{l}|^2 q^2 \right]^{1/2}, \end{aligned}$$

where  $q = M_2/M_1$  is the mass ratio and the angles are defined as



Figure 3.7: Comparison between the current final spin prediction and the actual total angular momentum of the binary system.

**MODEST-16** 



Figure 8. Mass of the runaway body,  $M_{\text{runaw}}$ , for each setup, averaged over 500 runs.  $M_{cl}(T = 0)$  is the total mass of the cluster at the time T = 0 and  $T_{rlx}(T = 0)$  the initial relaxation time of the cluster. The shaded area shows the standard deviation for the a = 0 case.

MO

#### Brem, Amaro-Seoane, Spurzem, MNRAS, 2013

Figure 9. Spin of the runaway body in each simulation, averaged over 500 runs. The shaded area shows the standard deviation for the a = 0 case. All initial spin setups lead to a similar evolution, except for the very first data point which is slightly higher for the maximally spinning initial conditions.





Post-Newtonian Dynamics Gravitational Wave Templates





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





#### **Example Detections in one of the Dragon models....**

#### Table header:

Status T[Gyr] Name1 Name2 M1[M\_sun] M2[M\_sun] a[AU] ecc Tm[Gyr] Tme[Gyr]

#### R7-IMF93 model

2 mergers in GC, 4 escapers:

1. There are two mergers in GCs [P] (merging time scale is very short)

P 2.32566 49 100229 25.6495 26.3923 12.51693 0.999867 6.18E-05 0.000124

P 1.54318 100237 100373 26.1701 21.932 8.93532 0.99996 3.06E-07 6.13E-07

There are two escaped mergers [E]: ('L' means the parameter before ejection)



	GW150914	GW151226	LVT151012
Source Mass 1	$36.2^{+5.2}_{-3.8}~M_{\odot}$	$14.2^{+8.3}_{-3.7} M_{\odot}$	$23^{+18}_{-6} \ M_{\odot}$
Source Mass 2	$29.1^{+3.7}_{-4.4}~M_{\odot}$	$7.5^{+2.3}_{-2.3} M_{\odot}$	$13^{+4}_{-5} \ M_{\odot}$
Luminosity Distance	$420^{+150}_{-180} \mathrm{Mpc}$	$440^{+180}_{-190} { m Mpc}$	$1000^{+500}_{-500} { m Mpc}$

Abbott, ..., DAB, et al. arXix 1606.04856

#### **GW Detection Frequency Time Diagram**

Top: Our simulation (Sobolenko , Veles, Wang, Berczik, Spurzem, et al. In prep Down: Abott et al. 2016 LIGO measurement



FIG. 1. The gravitational-wave event GW150914 observed by the LIGO Hanford (H1, left column panels) and Livingston (L1, right



FIG. 1: The multi-band GW astronomy concept. The violet lines are the total sensitivity curves (assuming two Michelson) of three eLISA configurations; from top to bottom N2A1, N2A2, N2A5 (from [11]). The orange lines are the current (dashed) and design (solid) aLIGO sensitivity curves. The lines in different blue flavours represent characteristic amplitude tracks of BHB sources for a realization of the *flat* population model (see main text) seen with S/N > 1 in the N2A2 configuration (highlighted as the thick eLISA middle curve), integrated assuming a five year mission lifetime. The light turquoise lines clustering around 0.01Hz are sources seen in eLISA with S/N < 5 (for clarity, we down-sampled them by a factor of 20 and we removed sources extending to the aLIGO band); the light and dark blue curves crossing to the aLIGO band are sources with S/N > 5 and S/N > 8 respectively in eLISA; the dark blue marks in the upper left corner are other sources with S/N > 8 in eLISA but not crossing to the aLIGO band within the mission lifetime. For comparison, the characteristic amplitude track completed by GW150914 is shown as a black solid line, and the chart at the top of the figure indicates the frequency progression of this particular source in the last 10 years before coalescence. The shaded area at the bottom left marks the expected confusion noise level produced by the same population model (median, 68% and 95% intervals are shown). The waveforms shown are second order post-Newtonian inspirals phenomenologically adjusted with a Lorentzian function to describe the ringdown.



Figure A1. A plot of characteristic strain against frequency for a variety of detectors and sources.



 Astrophysical High Precision N-Body – Star Clusters DRAGON simulations of low-density star cluster Need more Dragon simulations to study physics of rotation, binaries, high density, nuclear star clusters (Wang et al. 2015a, ApJ, 2015b, Cai et al. 2015, ApJS, Pang et al. 2015 RAA, Huang et al. 2015, RAA)
 Black Holes in Galactic Nuclei → see (Zhong et al. 2014, 2015, ApJ. Li et al. 2012 ApJ, 2015 subm. ApJ Khan et al. 2012, 2014 ApJ, Sobolenko et al. 2015, Berczik et al. 2016)
 Further Astrophysical Science Drivers:

Extragalactic and Massive Star Clusters IMBH Formation? Multiple Generations? Gravitational Waves in Pulsar Timing/eLISA/LIGO Radio Pulsars Accretion to central black holes





## **INVITATION/DISCUSSION**

- Building National and International Community on on Astrophysical GPU Supercomputing in China and Partner countries (e.g. South Africa, Pakistan, Chile...)
- Training and Teaching come to Beijing (NAOC) for testing and developing, or remote testing/running, or invite our experts for talks and hardware/software cooperation (regular schools and training workshops http://kiaa.pku.edu.cn/~kouwenhoven/nbody.html And GPU lectures.
- Relation to 'big data'
  common platforms
  for pathfinding/testing
  with simulations?



#### N-Body – Monte Carlo Comparison II Wang, Askar, Giersz, Spurzem, 2016, in prep.



Figure 2. The evolution of hard BHB ( $\tilde{a} < 100$  AU) numbers within core radii in R7-IMF93 ( $R_c = 2pc$ ) and R7-IMF01 ( $R_c = 3pc$ ). The blue curves show direct N-body (NBODY6++GPU) results and red curves show Monte-Carlo (MOCCA) results. These two curves have a same time resolution. The green curves show the same direct N-body result but higher time resolution.



Figure 3. The normalized distribution of hard BHB scaled-semimajor axises  $\tilde{a}$  ( $\tilde{a} < 100$  AU) within core radii in R7-IMF93 and R7-IMF01 models. The upper panels show the histograms and the lower panels show the cumulative distributions. To obtain better statistics, BHB data from snapshots of every 250 Myr between the ages of 1 Gyr and 12 Gyr are collected (totally 45 snapshots). The blue color indicates the direct N-body results and the red color indicates the Monte-Carlo results.