STROOPWAFEL: a Dutch cookie and an Adaptive Importance Sampling algorithm

Floor Broekgaarden

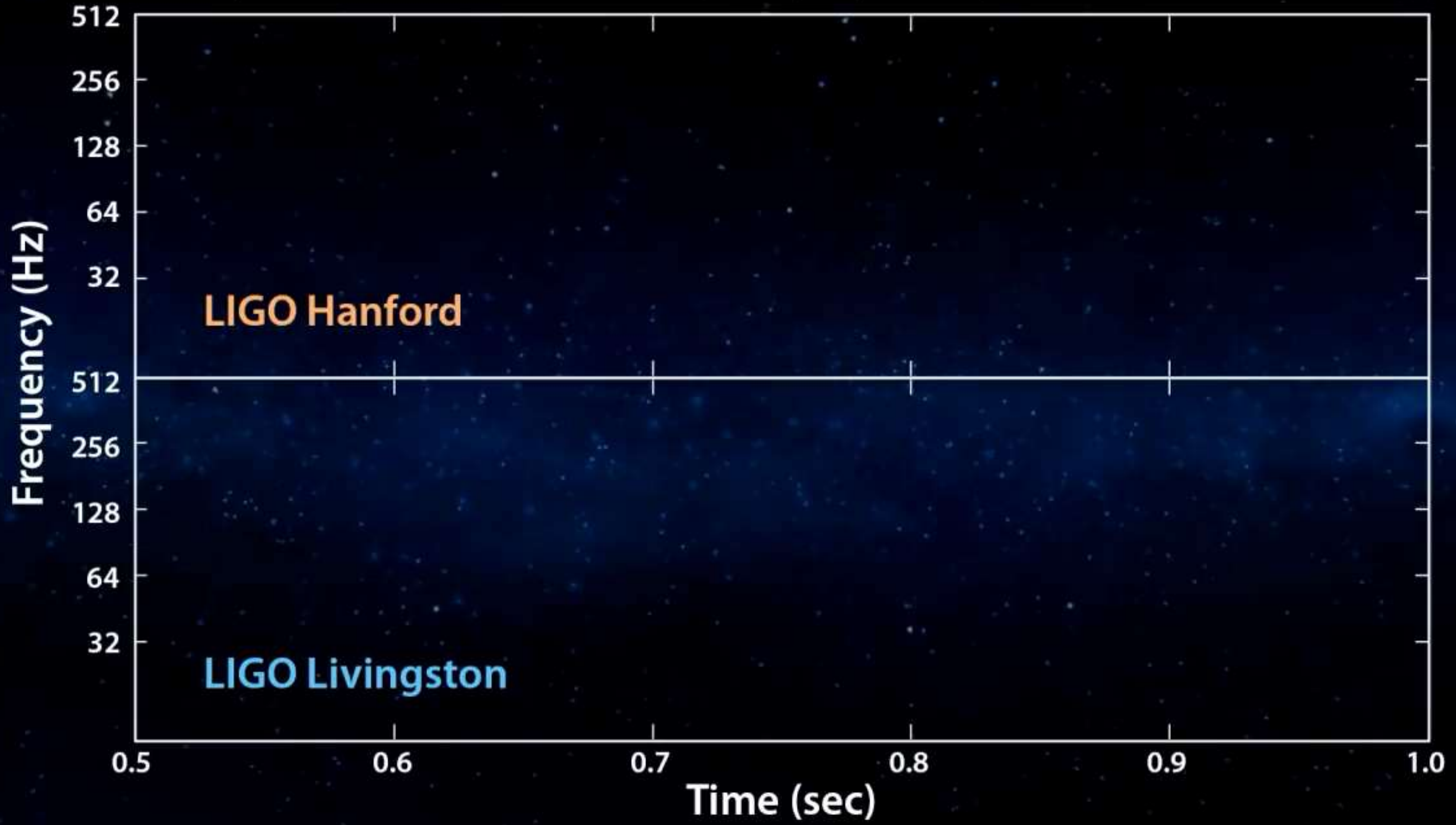
Center for Astrophysics | Harvard & Smithsonian

In collaboration with:

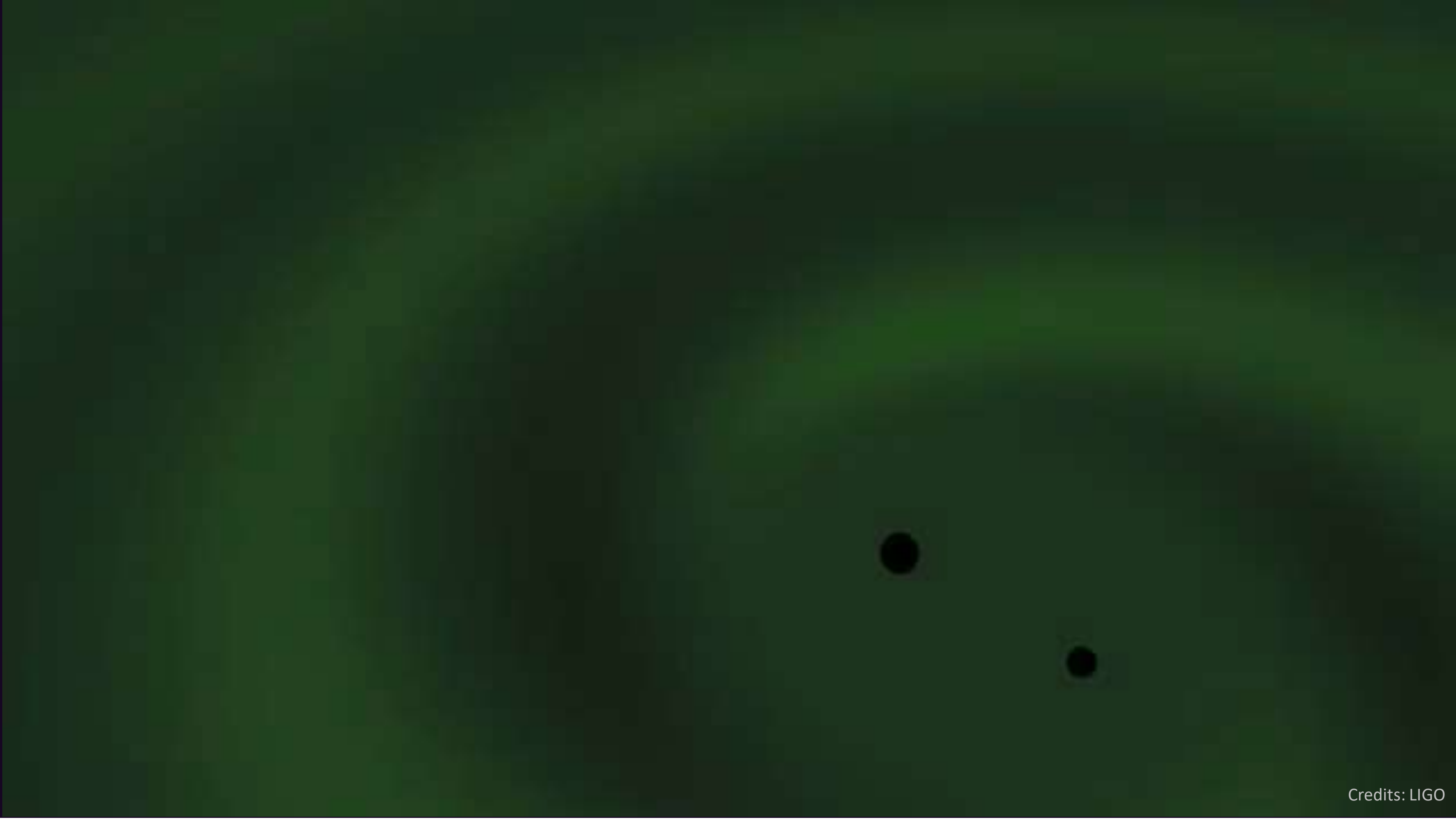
Jonathan Gair, Floris Kummer, Lokesh Khandelwal, Stephen Justham, Ilya Mandel, Selma de Mink, Luyau Lin, Coen Neijssel, Alejandro Vigna-Gomez, Simon Stevenson, Tom Wagg, Lieke van Son, Michelle Wassink, Poojan Agrawal, Serena Vinciguerra, Reinhold Willcox, Jeff Riley, Mike Lau and many others…

ICERM meeting | 20 November 2020

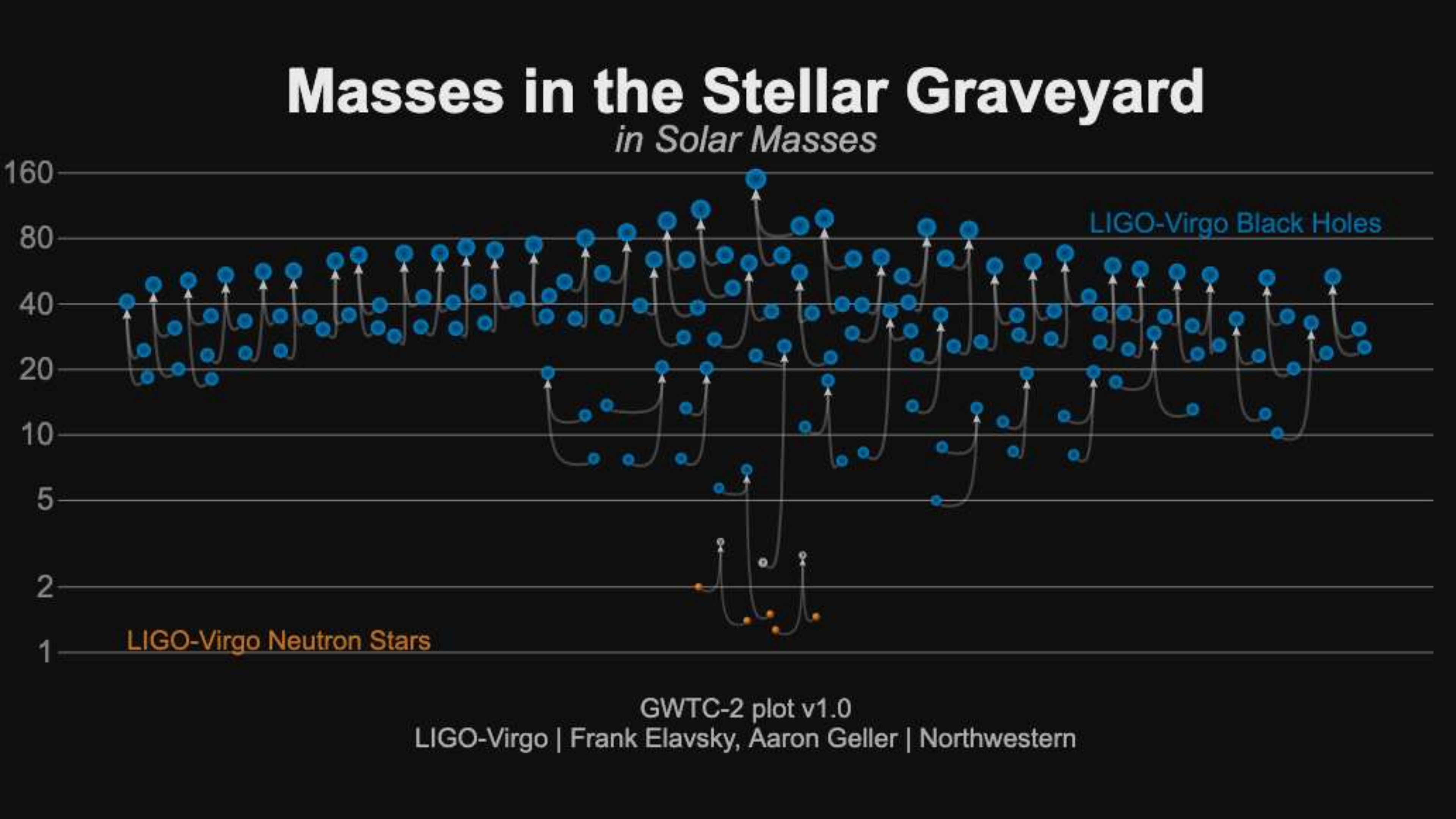
Statistical Methods for the Detection, Classification, and Inference of Relativistic Objects



Credits: LIGO

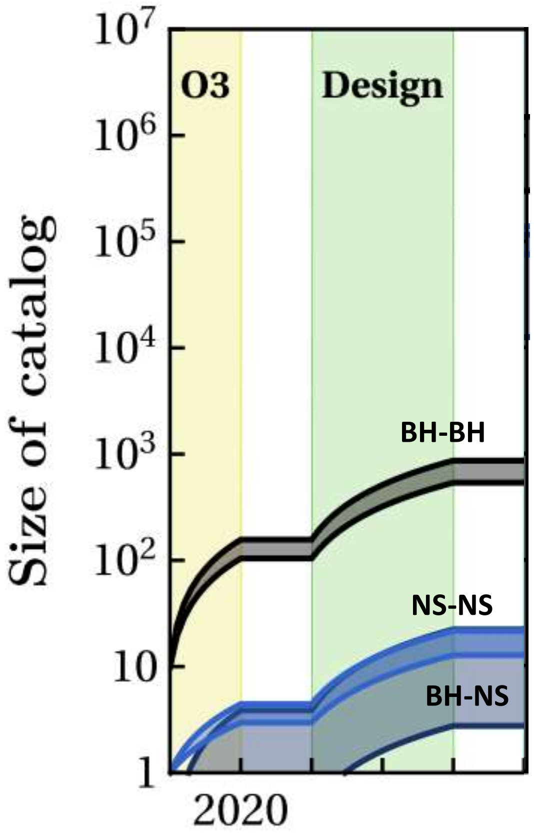


Credits: LIGO



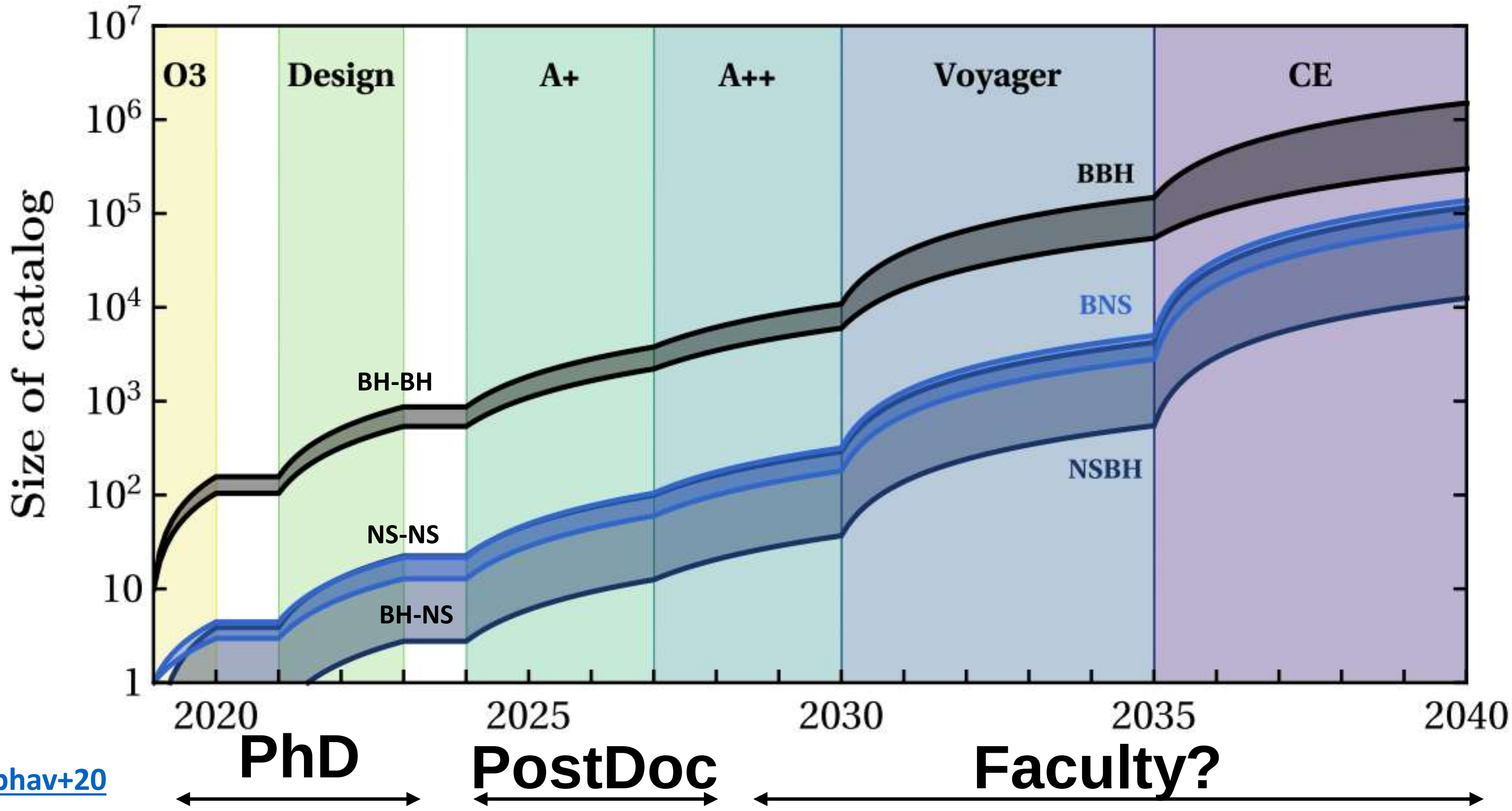
Masses in the Stellar Graveyard
in Solar Masses
160
80
40
20
10
5
2
1
LIGO-Virgo Black Holes
LIGO-Virgo Neutron Stars
GWTC-2 plot v1.0
LIGO-Virgo | Frank Elavsky, Aaron Geller | Northwestern

Building up a population of observations



Baibhav+20

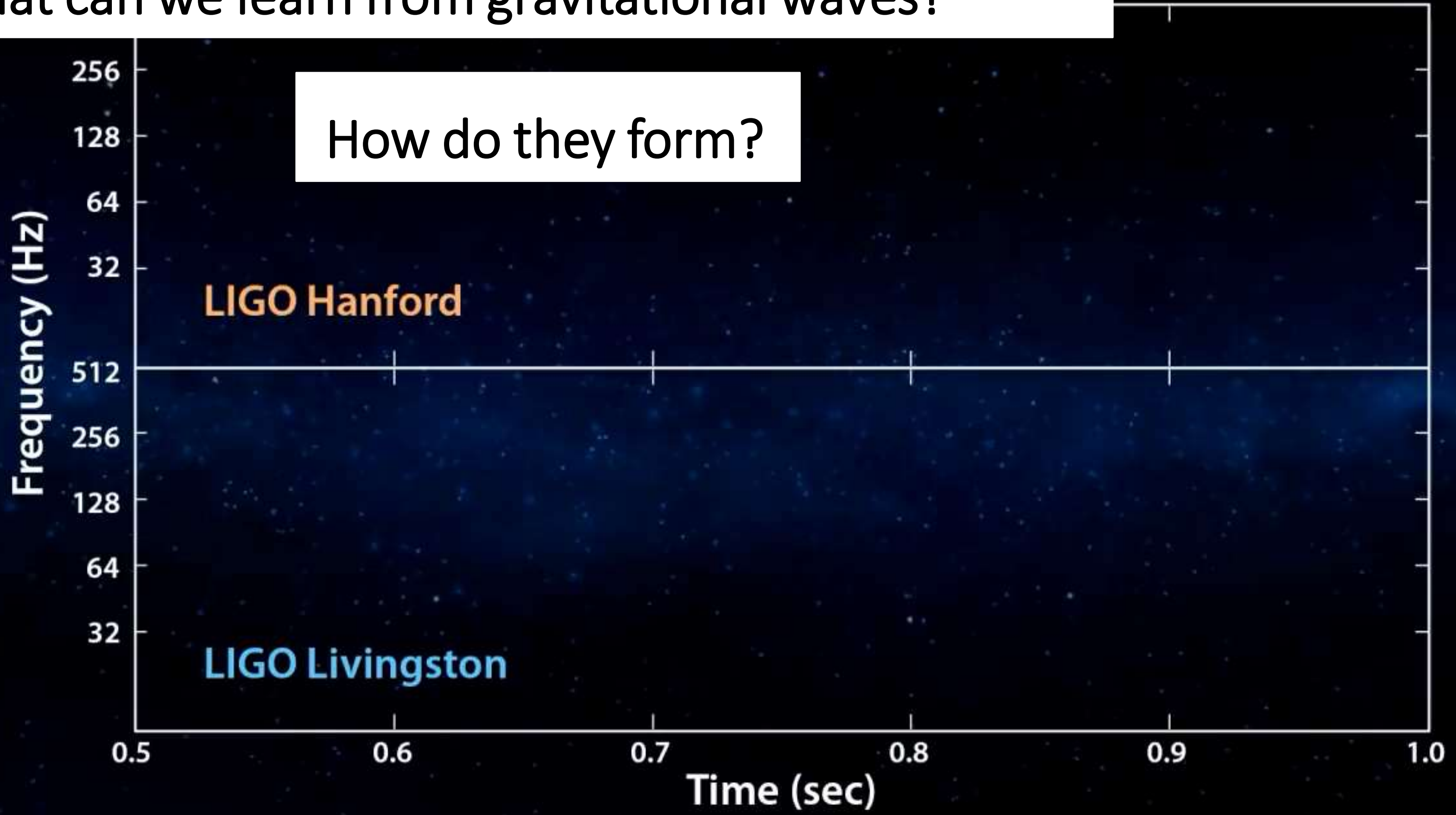
Building up a population of observations



Baibhav+20

What can we learn from gravitational waves?

How do they form?



Credits: LIGO

How do they form?

$z = 0$

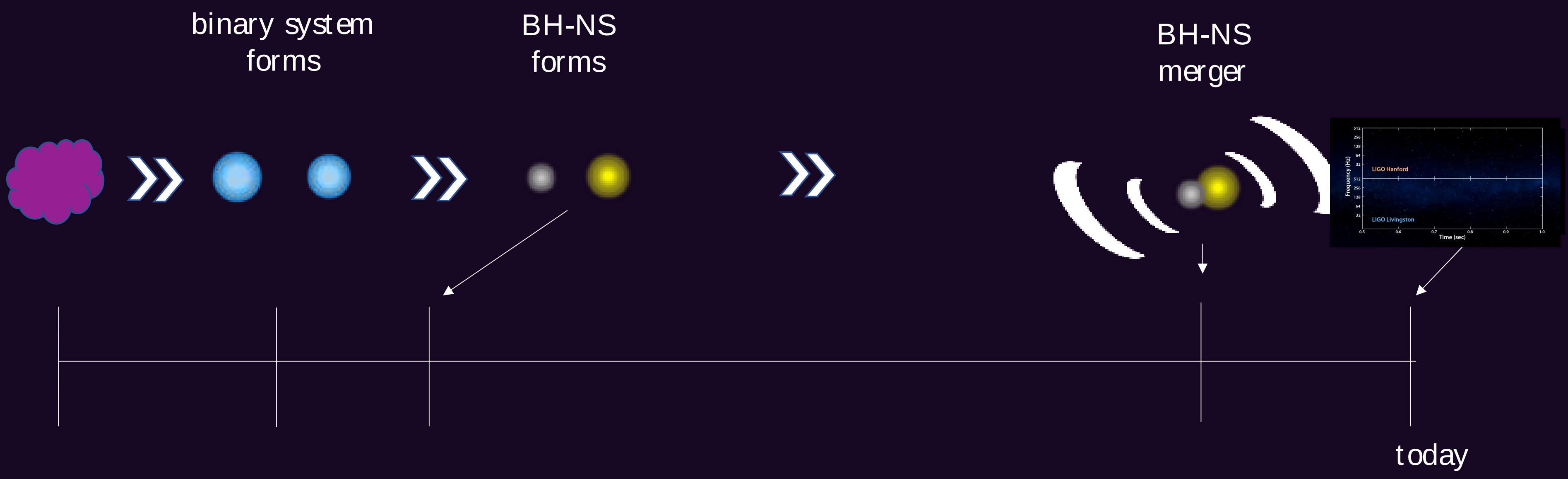


Image not to scale!

e.g. Paczynski+76, Smarr & Blandford+76

Rapid binary population synthesis

Stevenson+17, Barrett+18, Vigna-Gomez+18
Based on tracks from Hurley+00,02, Pols+98

Small images: Tauris+17

$$\mathbf{x}_\mathrm{i} = (m_{1,\mathrm{i}}, m_{2,\mathrm{i}}, a_\mathrm{i}, \ldots)$$

Initial conditions: mass 1, mass 2, separation, …

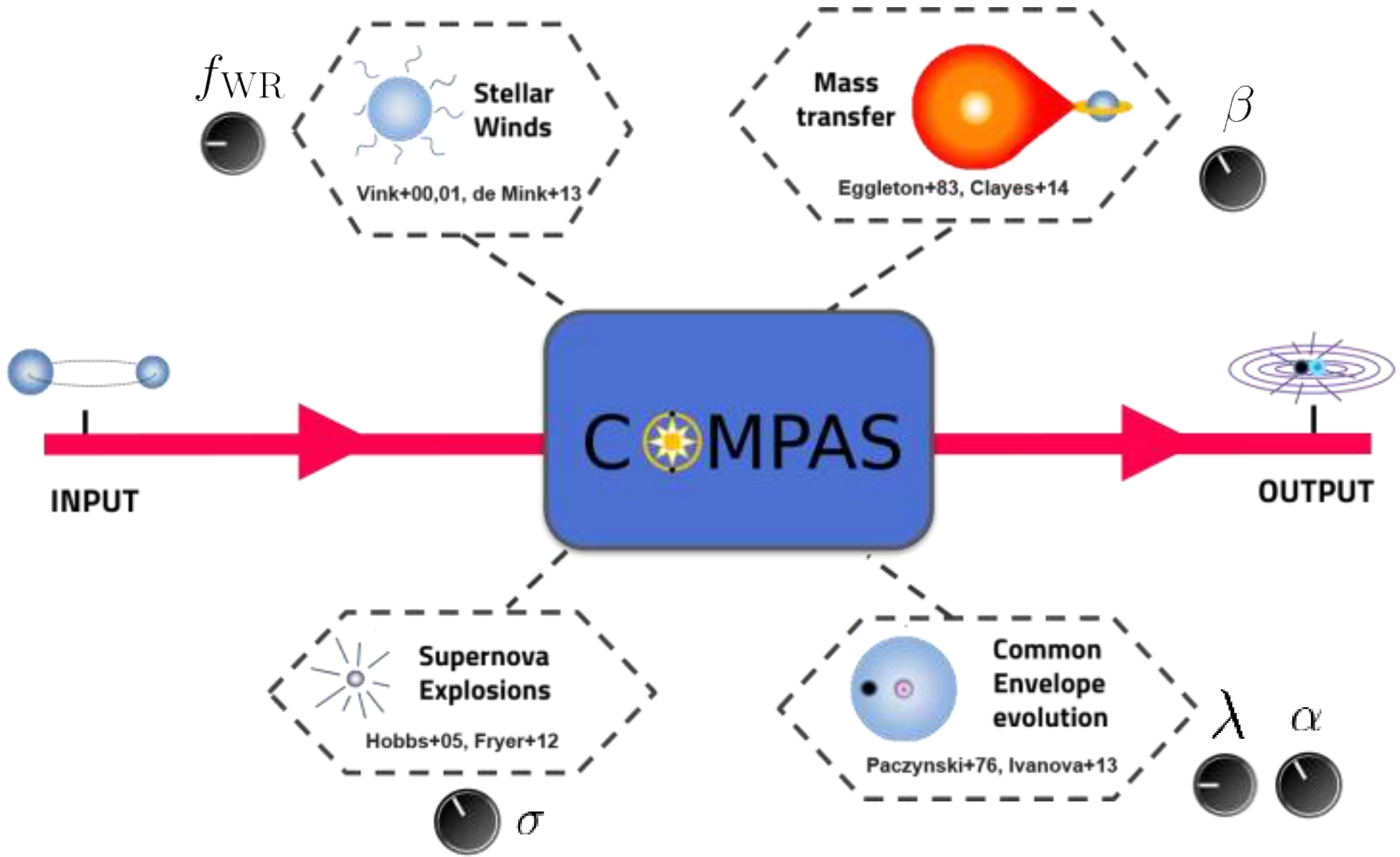
$$\mathbf{u}(\mathbf{x}_\mathrm{i}) = (m_{1,\mathrm{f}}, m_{2,\mathrm{f}}, \ldots)$$

final conditions: mass 1, mass 2, …

Rapid binary population synthesis

Stevenson+17, Barrett+18, Vigna-Gomez+18
Based on tracks from Hurley+00,02, Pols+98

Small images: Tauris+17



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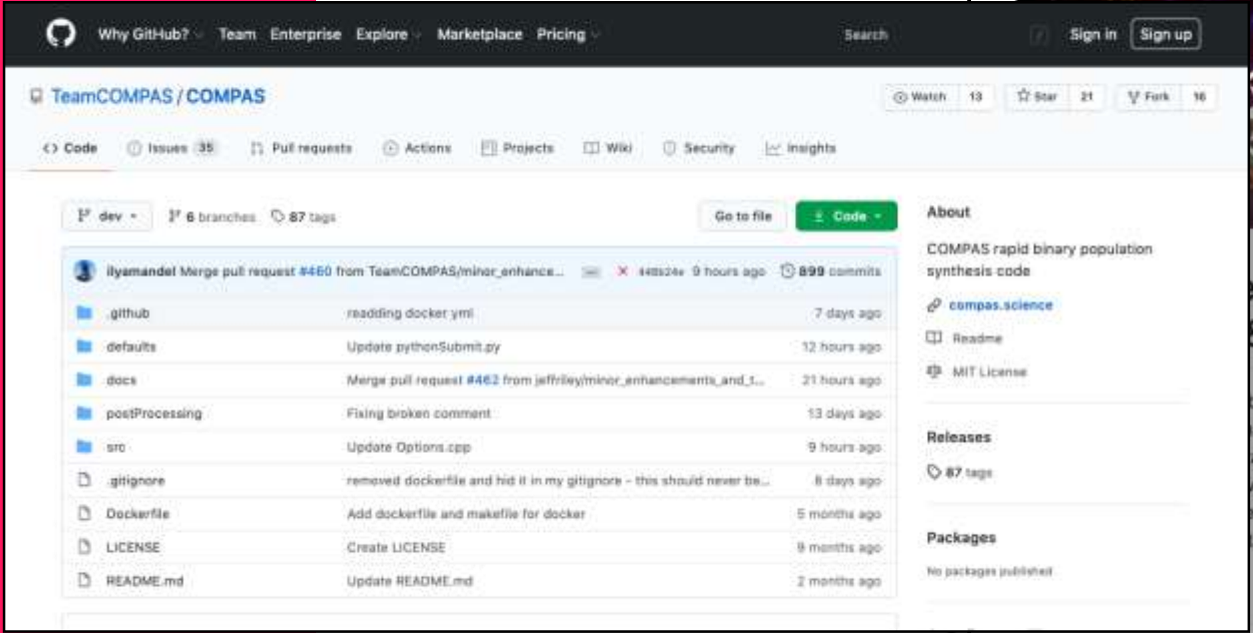
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TeamCOMPAS / COMPAS
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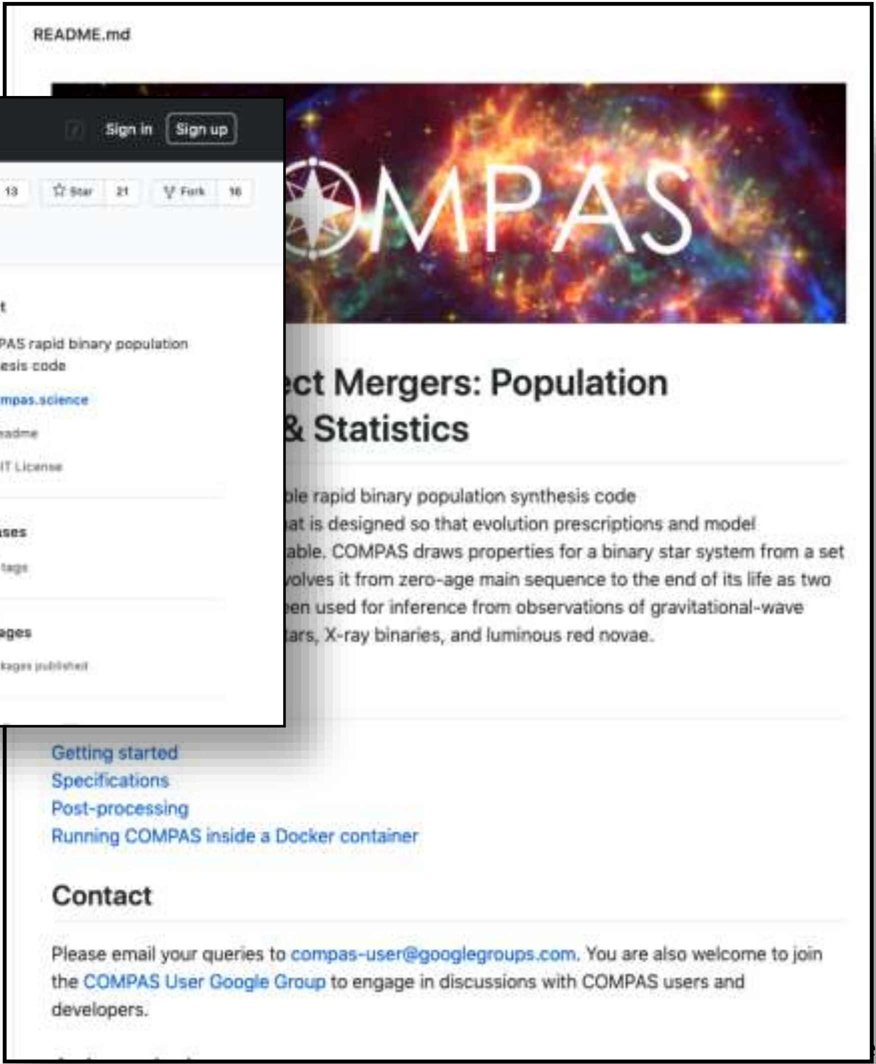
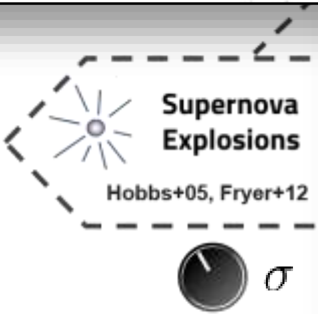
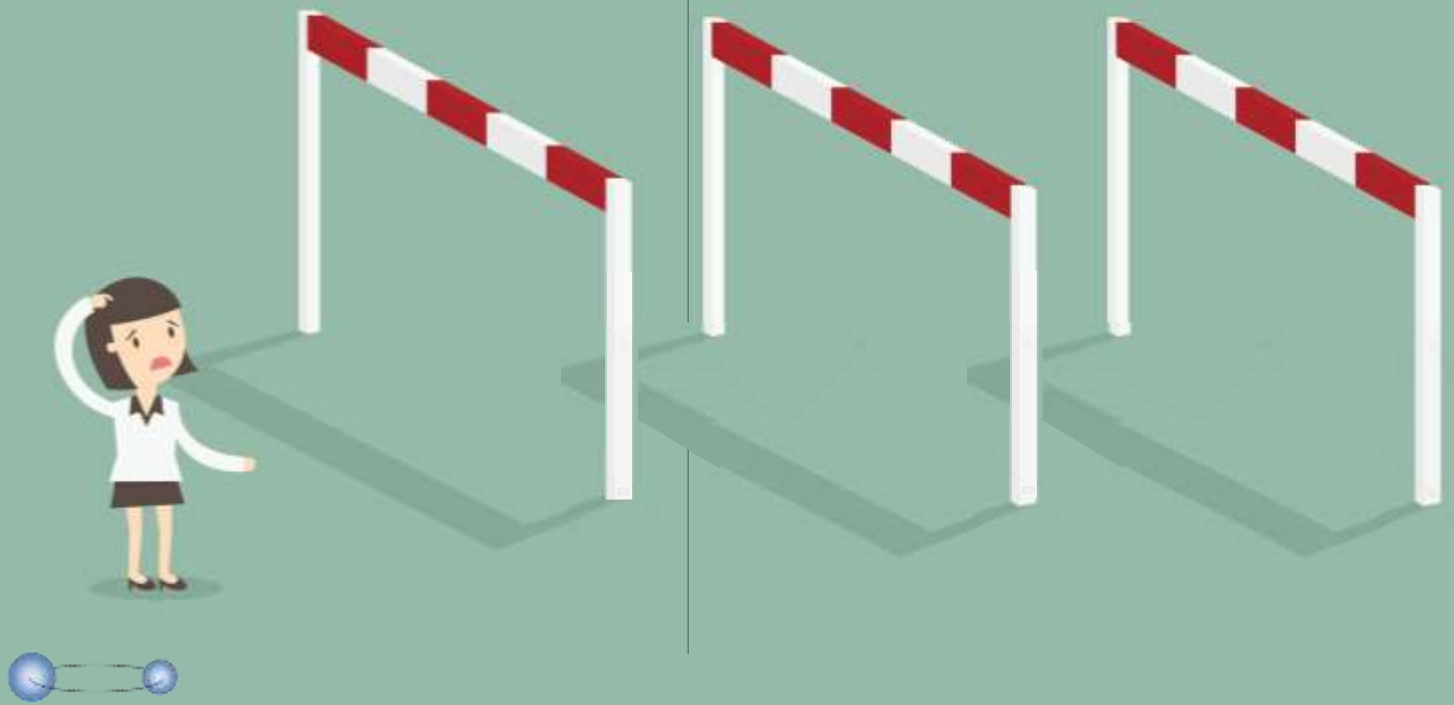
Star 21
Fork 16
Code
Issues 35
Pull requests
Actions
Projects
Wiki
Security
Insights
dev
6 branches
87 tags
Go to file
Code
ilyamandel Merge pull request #460 from TeamCOMPAS/minor_enhance...
9 hours ago
899 commits
.github
readding docker yml
7 days ago
defaults
Update pythonSubmit.py
12 hours ago
docs
Merge pull request #462 from jeffriley/minor_enhancements_and_f...
21 hours ago
postProcessing
Fixing broken comment
13 days ago
src
Update Options.cpp
9 hours ago
.gitignore
removed dockerfile and hid it in my gitignore - this should never be...
8 days ago
Dockerfile
Add dockerfile and makefile for docker
5 months ago
LICENSE
Create LICENSE
9 months ago
README.md
Update README.md
2 months ago
About
COMPAS rapid binary population synthesis code
compas.science
Readme
MIT License
Releases
87 tags
Packages
No packages published

README.md
COMPAS
ct Mergers: Population
& Statistics
ble rapid binary population synthesis code
at is designed so that evolution prescriptions and model
able. COMPAS draws properties for a binary star system from a set
volves it from zero-age main sequence to the end of its life as two
en used for inference from observations of gravitational-wave
ars, X-ray binaries, and luminous red novae.
Getting started
Specifications
Post-processing
Running COMPAS inside a Docker container
Contact
Please email your queries to compas-user@googlegroups.com. You are also welcome to join the COMPAS User Google Group to engage in discussions with COMPAS users and developers.

Supernova
Explosions
Hobbs+05, Fryer+12
σ

cartoon from DooderVector/everypixel

3 computational challenges

1 Simulating populations



Cost:

~1 sec

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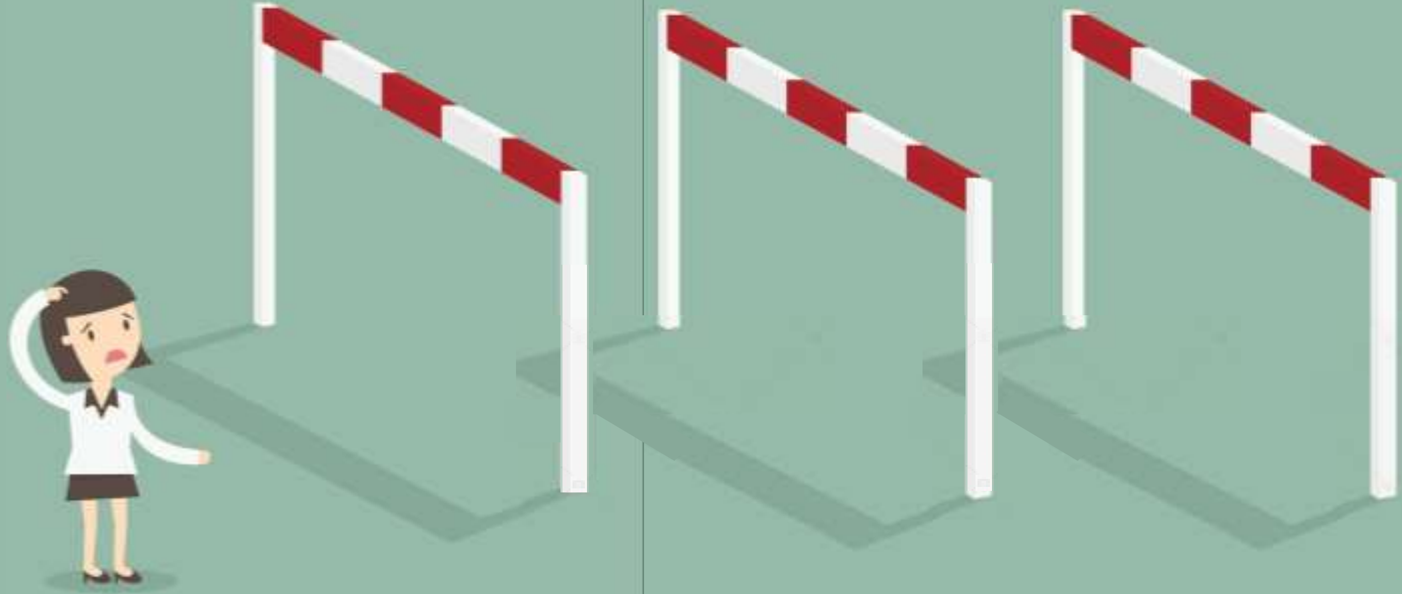
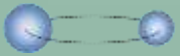
3 computational challenges

1 Simulating populations

2 Testing physics





Cost: ~ 1 sec $\times\ 10^6$

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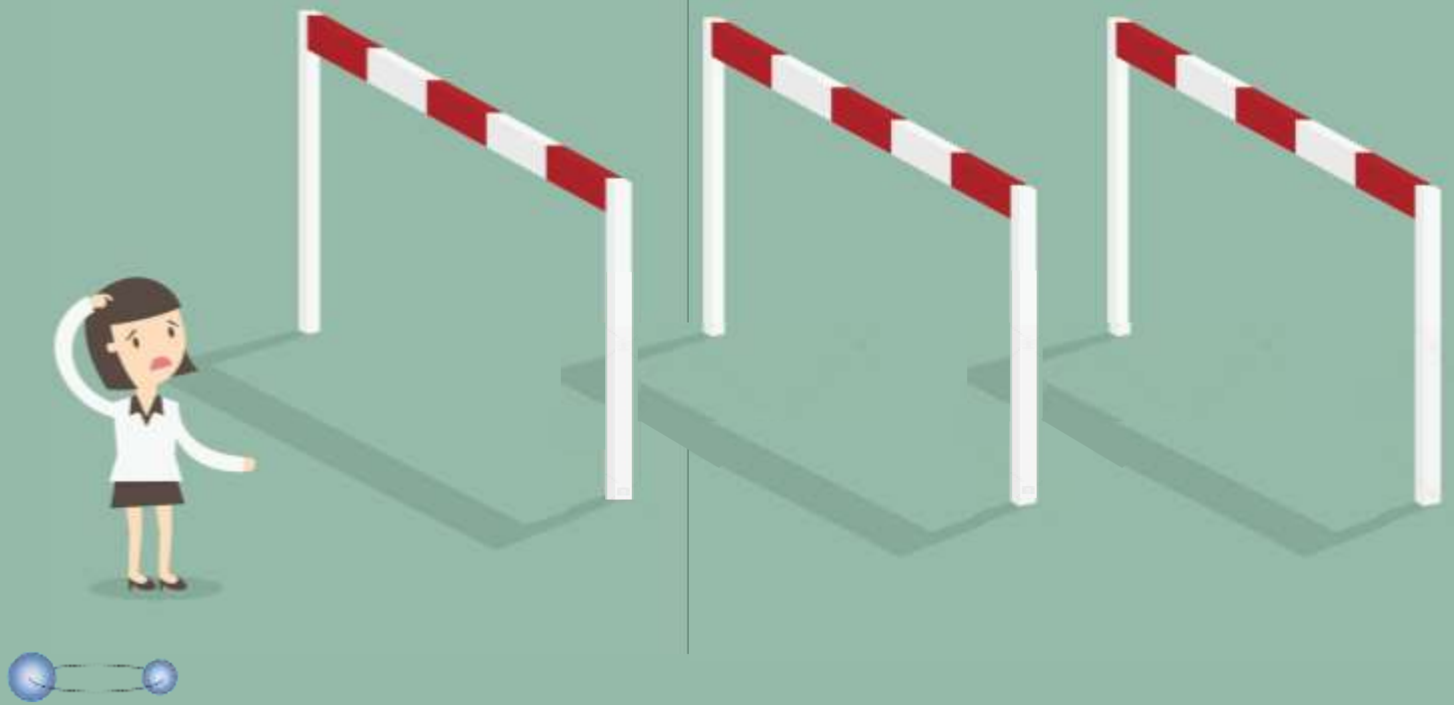
3 computational challenges



1 Simulating populations

2 Testing physics

3 Rare events

Cost: ~ 1 sec $\times 10^6$ $\times 10 - 10^6$

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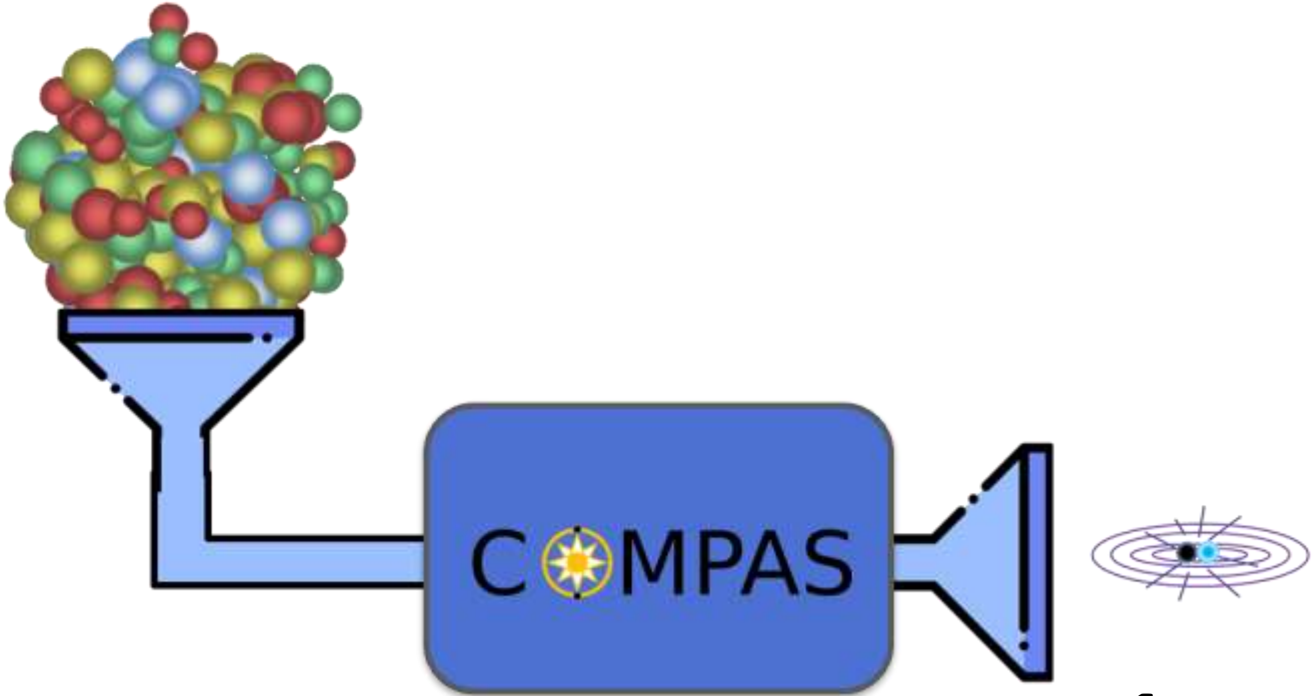
3 Rare events:

1000 binaries



only ~1

BH-NS merger!

E.g. Belczynski+02

3 computational challenges

1 Simulating populations

2 Testing physics

3 Rare events

Cost: ~ 1 sec $\times 10^6$ $\times 10 - 10^6$ $\times 10 - 10^3$

$\sim 3 - 3 \times 10^6$ years computing time

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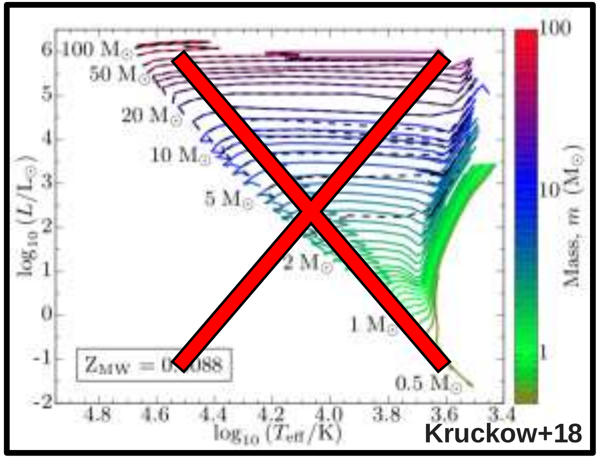
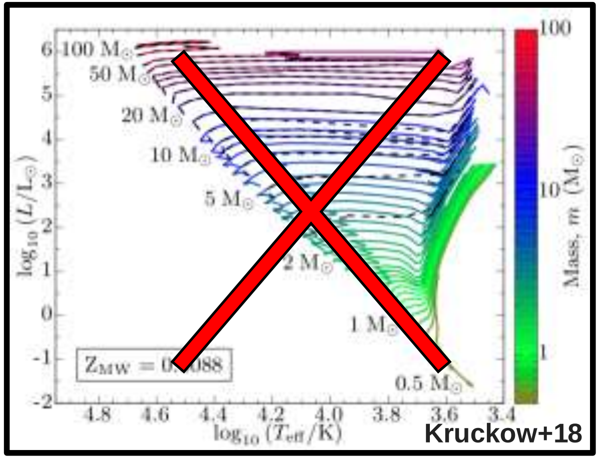
Current binary population synthesis models pay a high price…

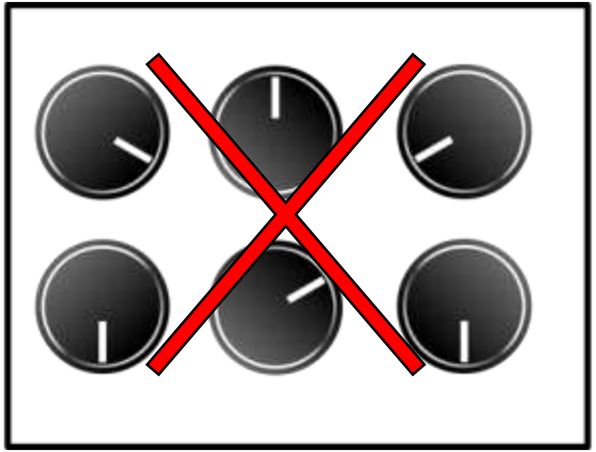


Do not include detailed prescriptions

Current binary population synthesis models pay a high price…

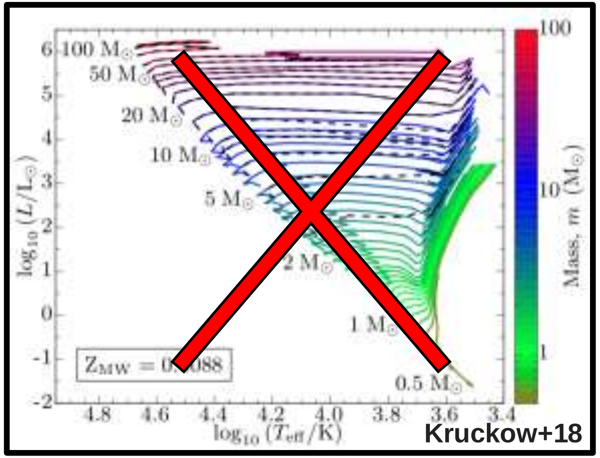


Do not include detailed prescriptions

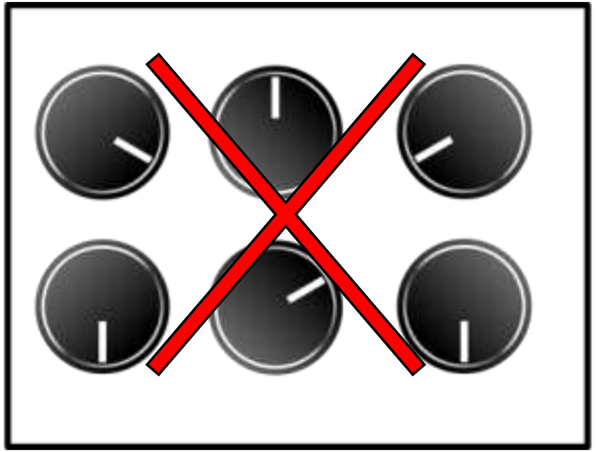


Perform only a small parameter study

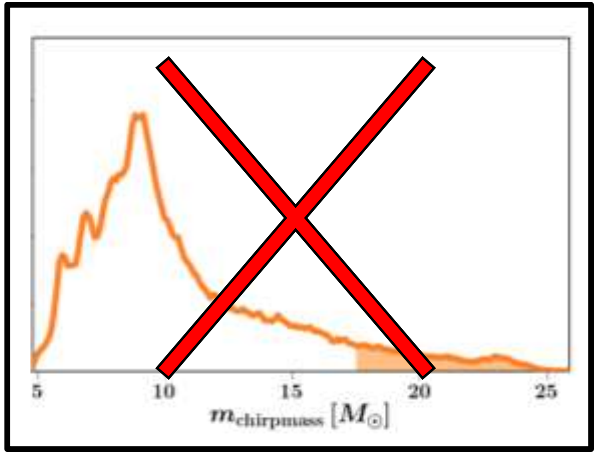
Current binary population synthesis models pay a high price…



Do not include detailed prescriptions



Perform only a small parameter study



Do not explore tails of distributions

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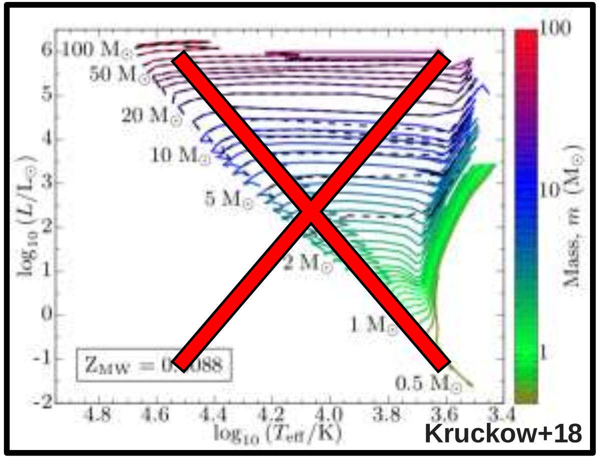
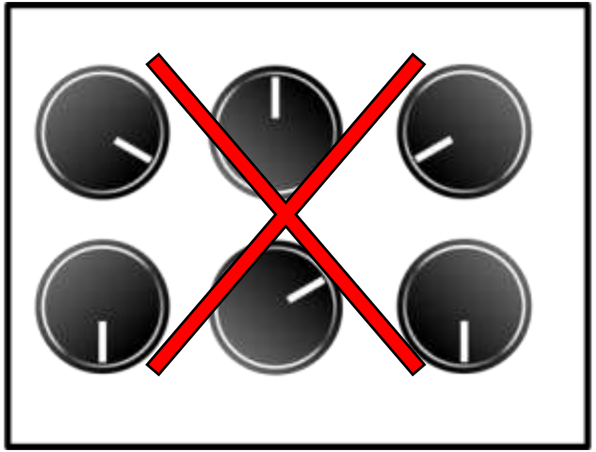
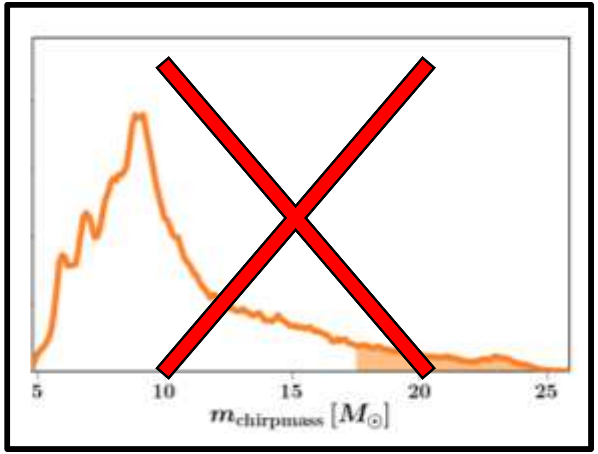
C… opulation synthesis models pay a high price…



Do not include detailed prescriptions



Perform only a small parameter study



Do not explore tails of distributions

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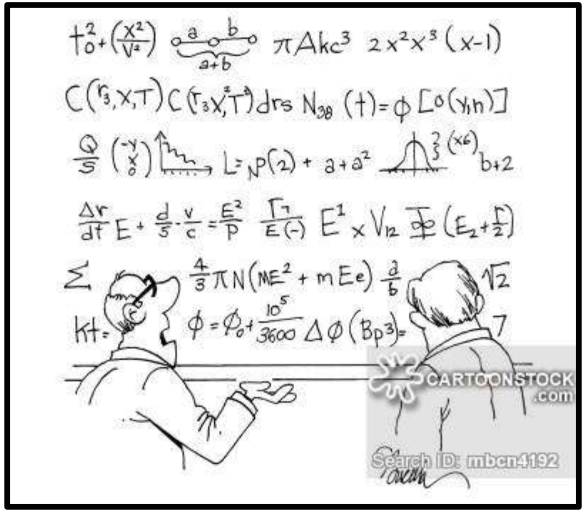
Previous work

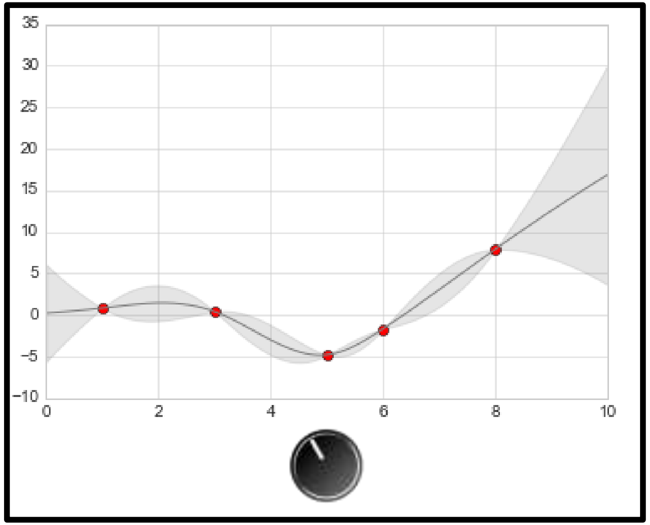
Analytical formalisms

Kolb 1993, Politano 1996, Kalogera 1996
Kalogera&Webbink 1998, Kalogera+2000



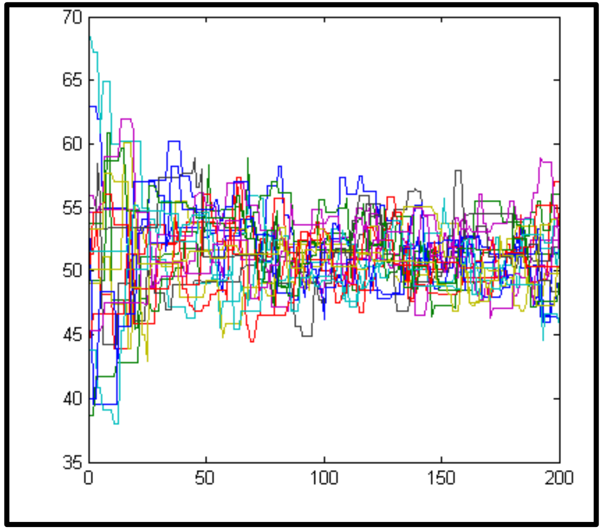
Emulators (GPR)

Barret+2017, Taylor & Gerosa 2018,
Wong & Gerosa 2019



Markov Chain Monte Carlo

Andrews+2017; (dart_board)



We present:

(drum roll)

New sampling algorithm:

Simulating The Rare Outcomes Of Populations With AIS For Efficient Learning

STROOPWAFEL

Adaptive Importance Sampling (AIS)

Marin+06, Douc+07, Owen+09, Martino+15
AIS: Torrie & Valleau 1977, Hesterberg 1995, Cappe+2004, Pennanen & Koivu 2006, Cornuet+2012, Ortiz & Pack Kaelbling (2013), …

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New sampling algorithm:

Simulating The Rare Out

Wi

Adaptive In

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MONTHLY NOTICES

Volume 490, Issue 4
December 2019

Article Contents

STROOPWAFEL: simulating rare outcomes from astrophysical populations, with application to gravitational-wave sources*

Floor S Broekgaarden ✉, Stephen Justham, Selma E de Mink, Jonathan Gair, Ilya Mandel, Simon Stevenson, Jim W Barrett, Alejandro Vigna-Gómez, Coenraad J Neijssel

Monthly Notices of the Royal Astronomical Society, Volume 490, Issue 4, December 2019, Pages 5228–5248, https://doi.org/10.1093/mnras/stz2558
Published: 27 September 2019 **Article history** ▾

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ABSTRACT

Gravitational-wave observations of double compact object (DCO) mergers are providing new insights into the physics of massive stars and the evolution of binary systems. Making the most of expected near-future observations for understanding stellar physics will rely on comparisons with binary population

), ...

New sampling algorithm:

Simulating The Rare Outcomes Of Populations With AIS For Efficient Learning

Adaptive Importance Sampling (AIS)

Marin+06, Douc+07, Owen+09, Martino+15
AIS: Torrie & Valleau 1977, Hesterberg 1995, Cappe+2004, Pennanen & Koivu 2006, Cornuet+2012, Ortiz & Pack Kaelbling (2013), …

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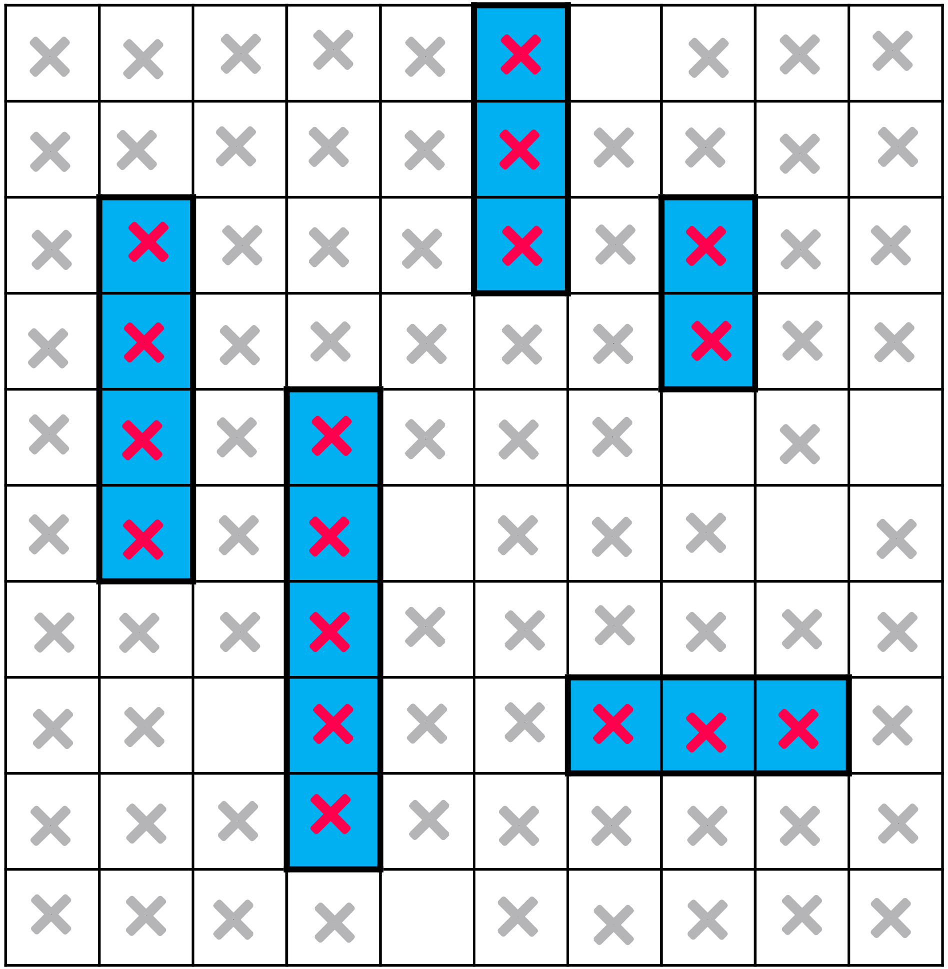
Traditional models use *"random shooting"*:

requires

< 96 >

shots

to complete the game



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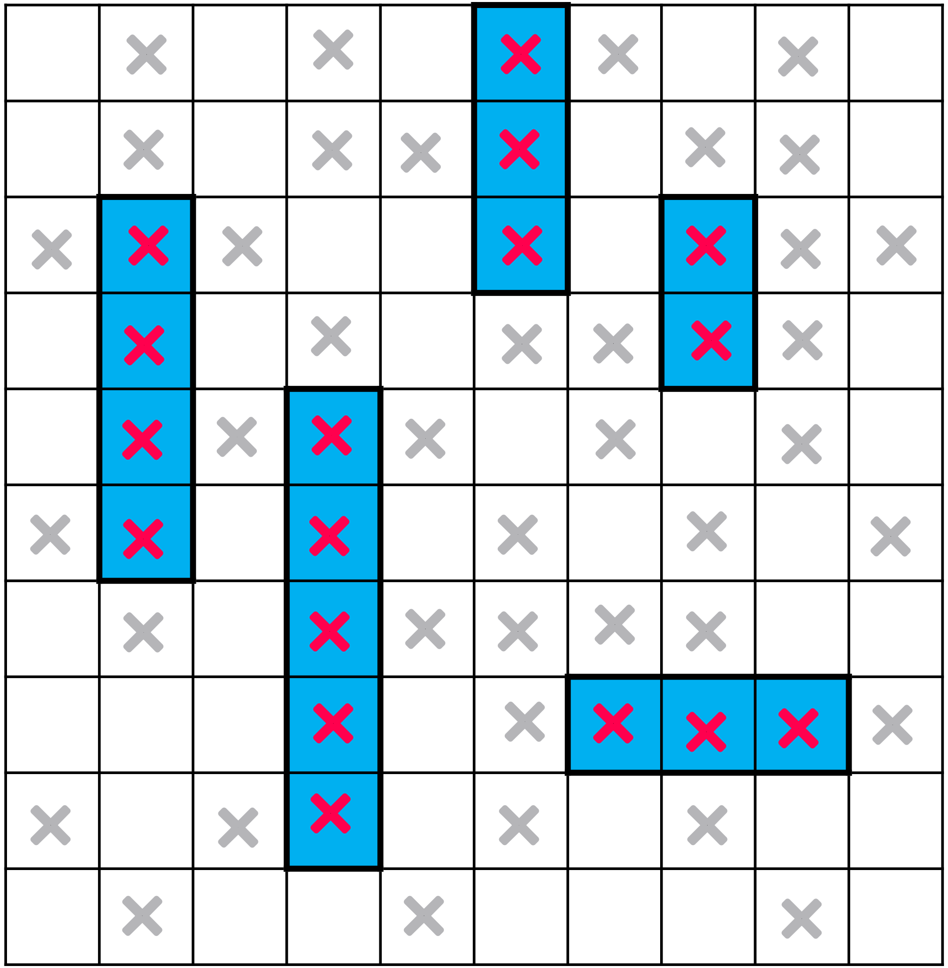
STROOPWAFEL
uses *“explore/refine”*:

requires

<??>

shots

to complete the game



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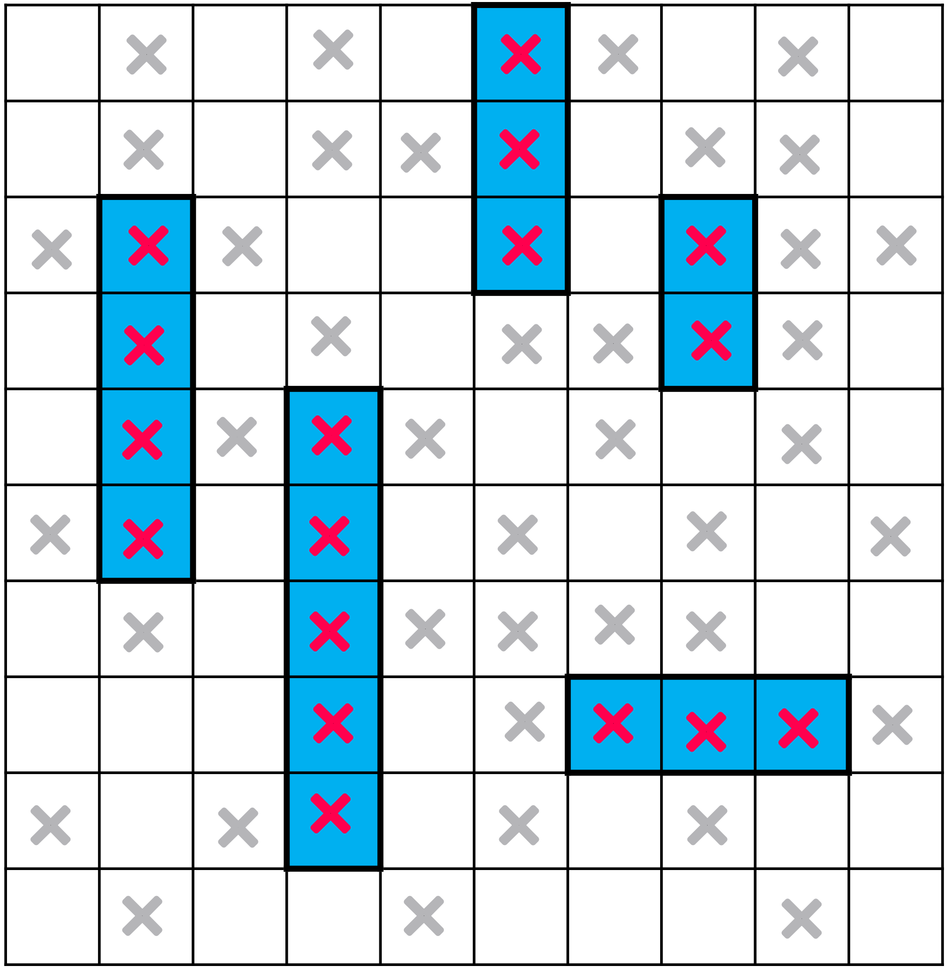
STROOPWAFEL
uses *“explore/refine”*:

requires

< 65 >

shots

to complete the game



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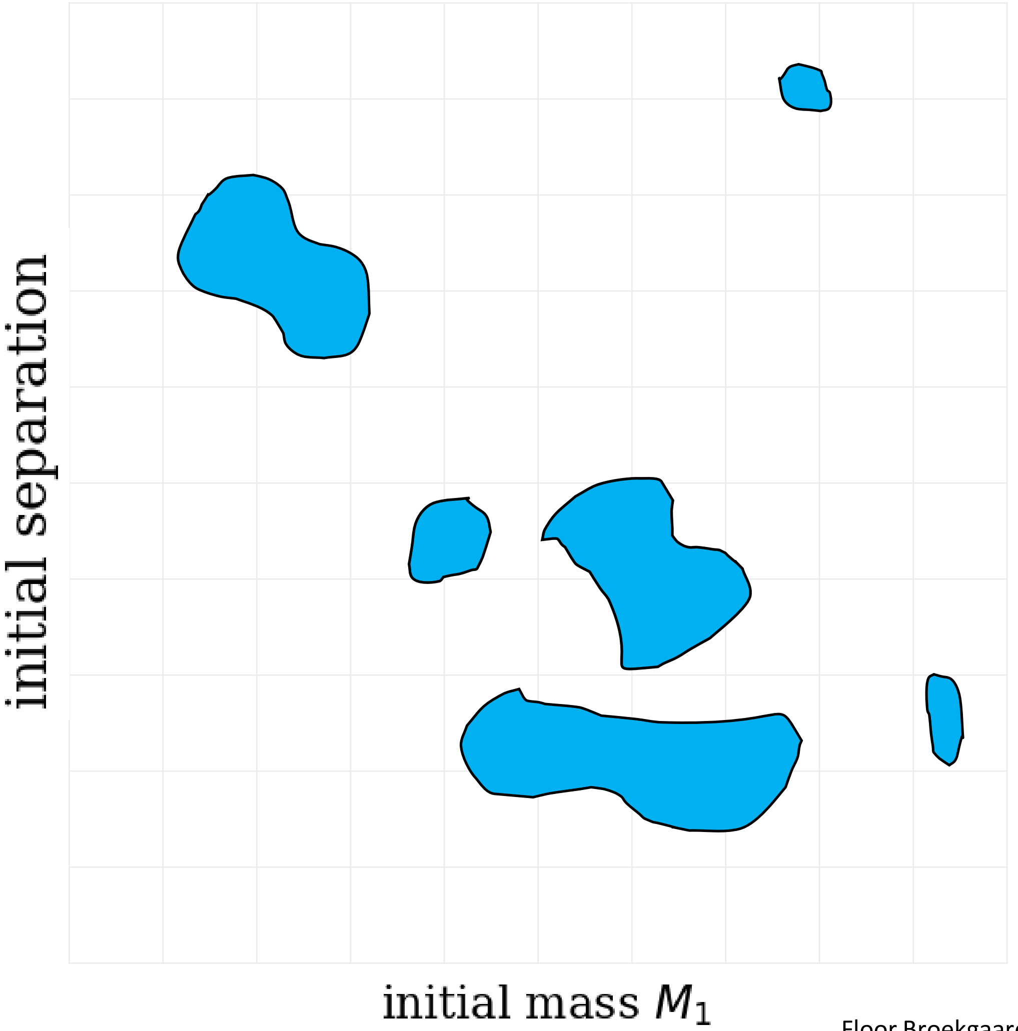
Binary population synthesis:

- High-dimensional space,
- Unknown “islands” that form, e.g., BH-BH mergers
- unknown “rate” $\sim \frac{1}{1000}$



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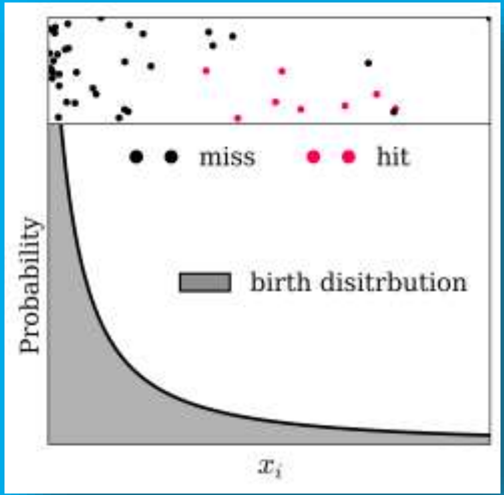
prior

$$\pi(\boldsymbol{x}_i) = \pi(m_{1,i}, m_{2,i}, a_i, \cdots)$$

1) Exploring phase



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prior

$$\pi(\boldsymbol{x}_i) = \pi(m_{1,i}, m_{2,i}, a_i, \cdots)$$

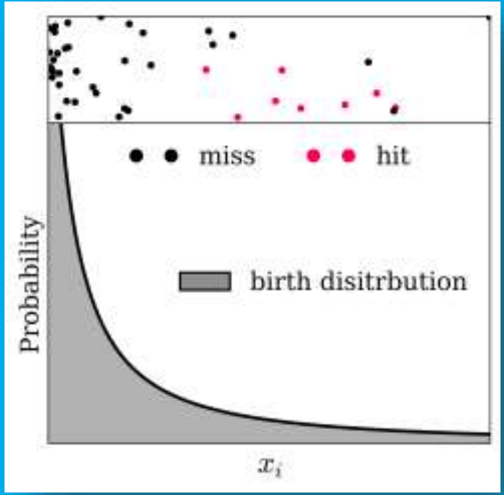
Gaussian
around hits

$$q(\boldsymbol{x}) = \frac{1}{N_{\mathrm{T,expl}}} \sum_{k=1}^{N_{\mathrm{T,expl}}} q_k(\boldsymbol{x}; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

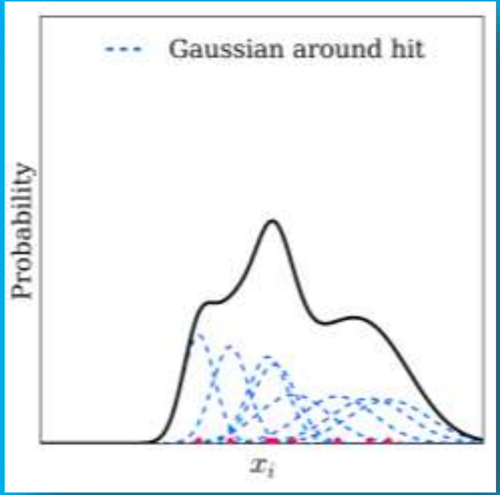
$$\sigma_{j,k} = \kappa \frac{1}{\pi_j(x_k) N_{\mathrm{expl}}^{1/d}},$$

Gaussian width

1) Exploring phase



2) Create adapted distribution



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$$\pi(\boldsymbol{x}_i) = \pi(m_{1,i}, m_{2,i}, a_i, \cdots)$$

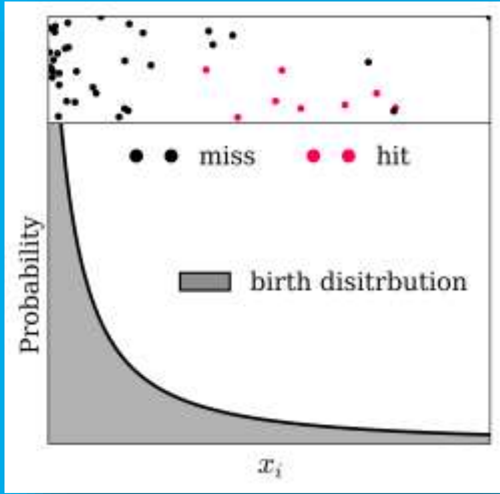
Gaussian around hits

$$q(\boldsymbol{x}) = \frac{1}{N_{\mathrm{T,expl}}} \sum_{k=1}^{N_{\mathrm{T,expl}}} q_k(\boldsymbol{x}; \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

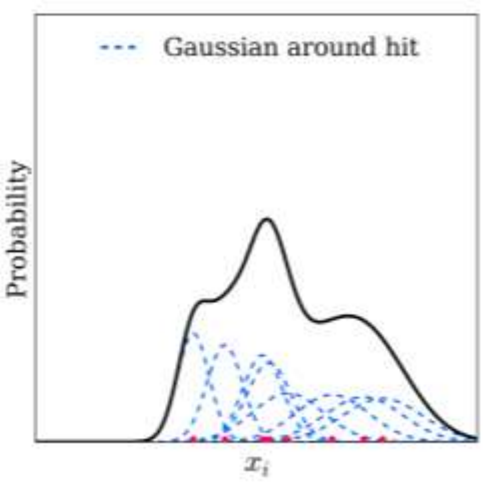
Gaussian width

$$\sigma_{j,k} = \kappa \frac{1}{\pi_j(x_k) N_{\mathrm{expl}}^{1/d}},$$

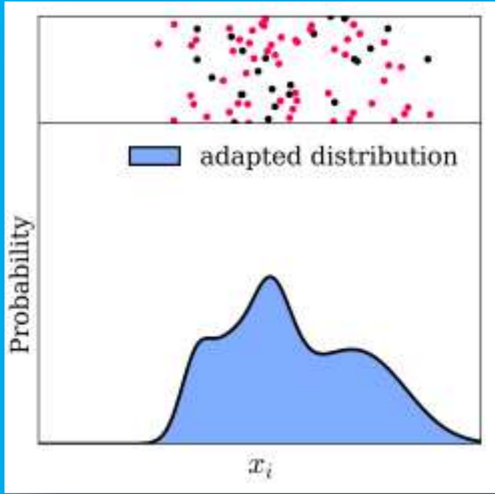
1) Exploring phase



2) Create adapted distribution



3) Refinement phase



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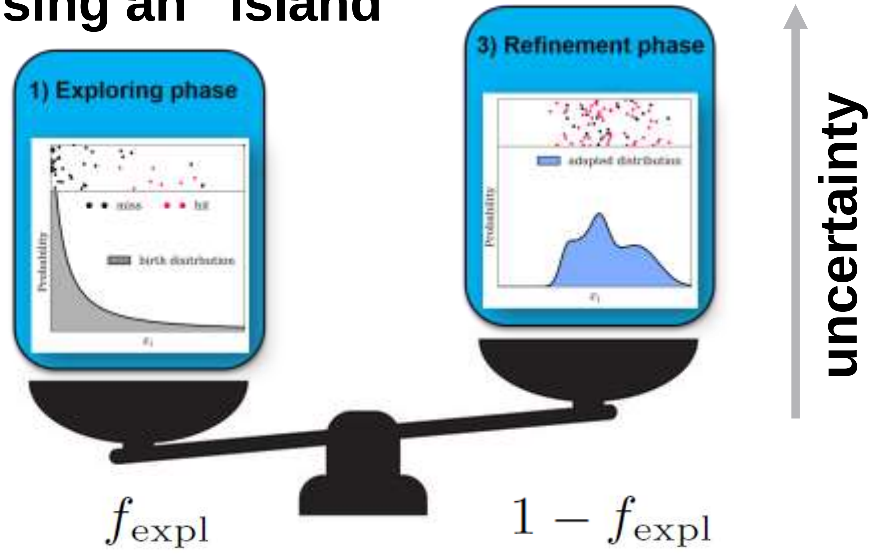
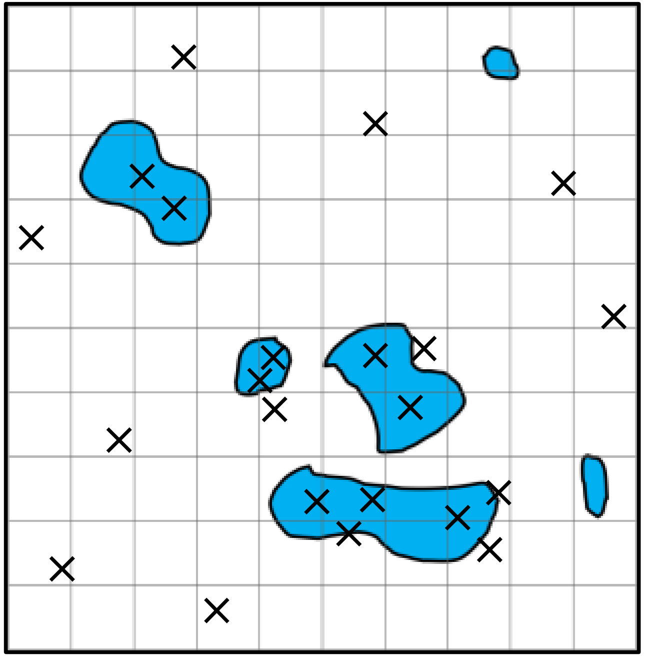
When to switch from exploring to refinement?

Getting more "hits"

Missing an "island"





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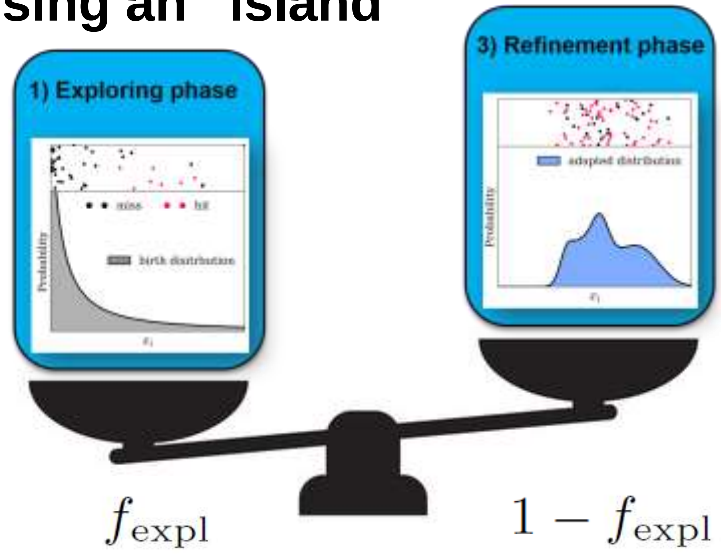

Alternative to e.g. Effective Sample Size (ESS) Hesterberg 1995; Liu 2008

Uncertainty from refining

$$f_{\mathrm{expl}} = 1 - \frac{z_1(\sqrt{1-z_1} - \sqrt{z_2})}{\sqrt{1-z_1}(\sqrt{z_2(1-z_1)} + z_1)}$$

uncertainty from missing an island

Ingredients

- 6 different target populations

- 3 parameters:
  m1, m2 & separation

- traditional vs STROOPWAFEL sampling

Simulation	Target subpopulation
1	All DCO mergers in a Hubble time
2	BH–BH mergers in a Hubble time
3	BH–NS mergers in a Hubble time
4	NS–NS mergers in a Hubble time
5	BH–BH mergers $m_{\rm tot} > 50\,{\rm M}_{\odot}$
6	NS–NS mergers with $t_{\rm coal} < 50\,{\rm Myrs}$

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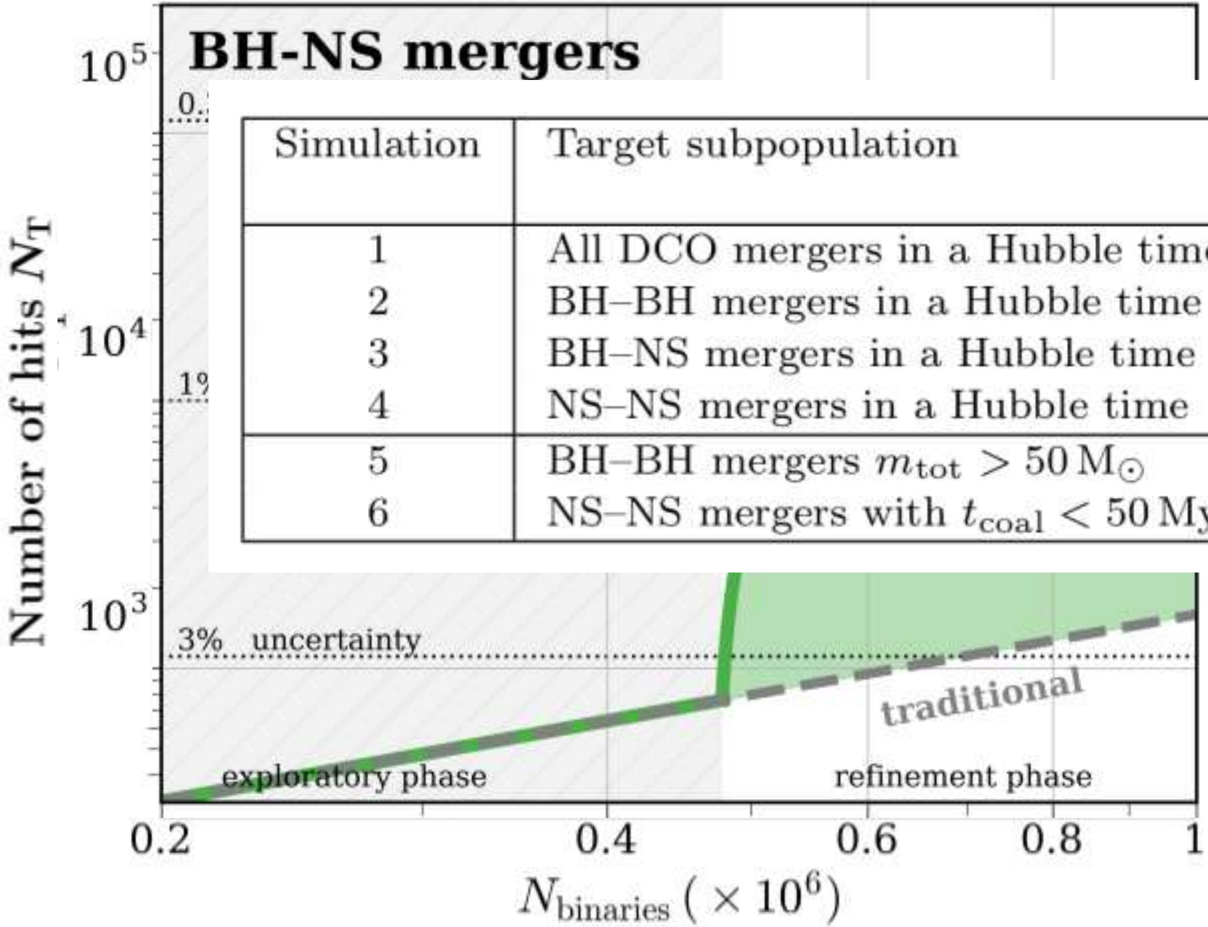
Higher efficiency



Simulation	Target subpopulation	gain
1	All DCO mergers in a Hubble time	35×
2	BH–BH mergers in a Hubble time	53×
3	BH–NS mergers in a Hubble time	39×
4	NS–NS mergers in a Hubble time	45×
5	BH–BH mergers $m_{\mathrm{tot}} > 50\,\mathrm{M}_\odot$	202×
6	NS–NS mergers with $t_{\mathrm{coal}} < 50\,\mathrm{Myrs}$	24×

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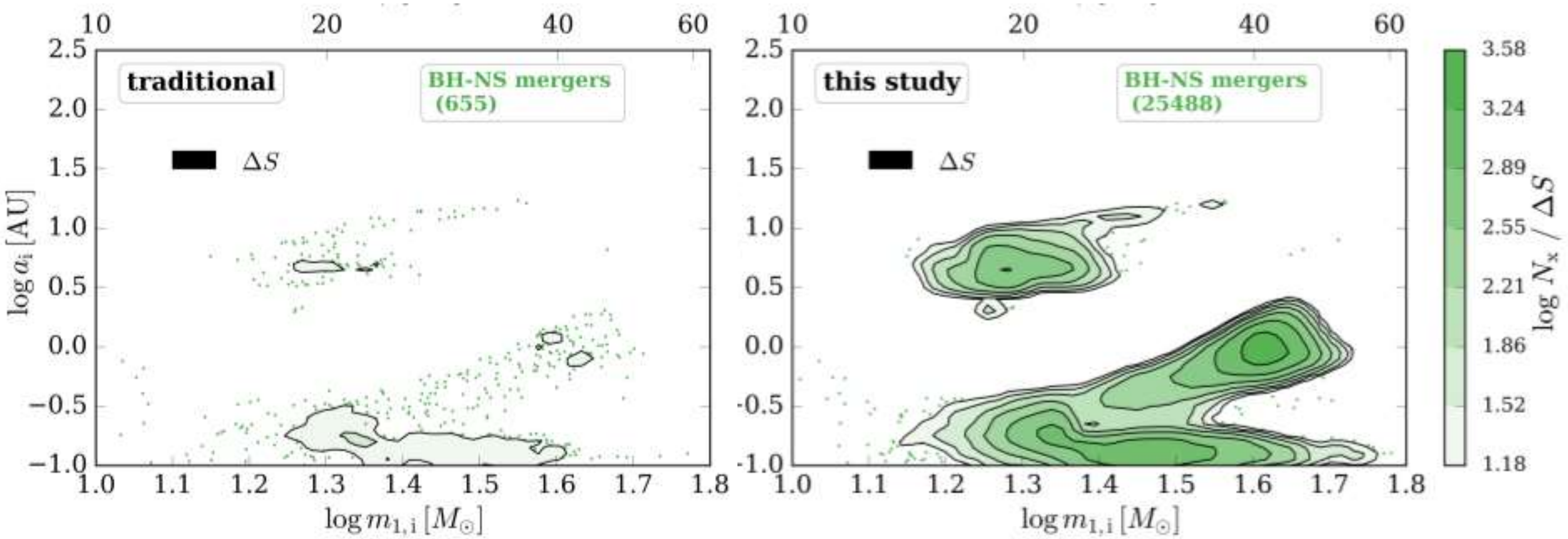
Higher resolution on input parameters



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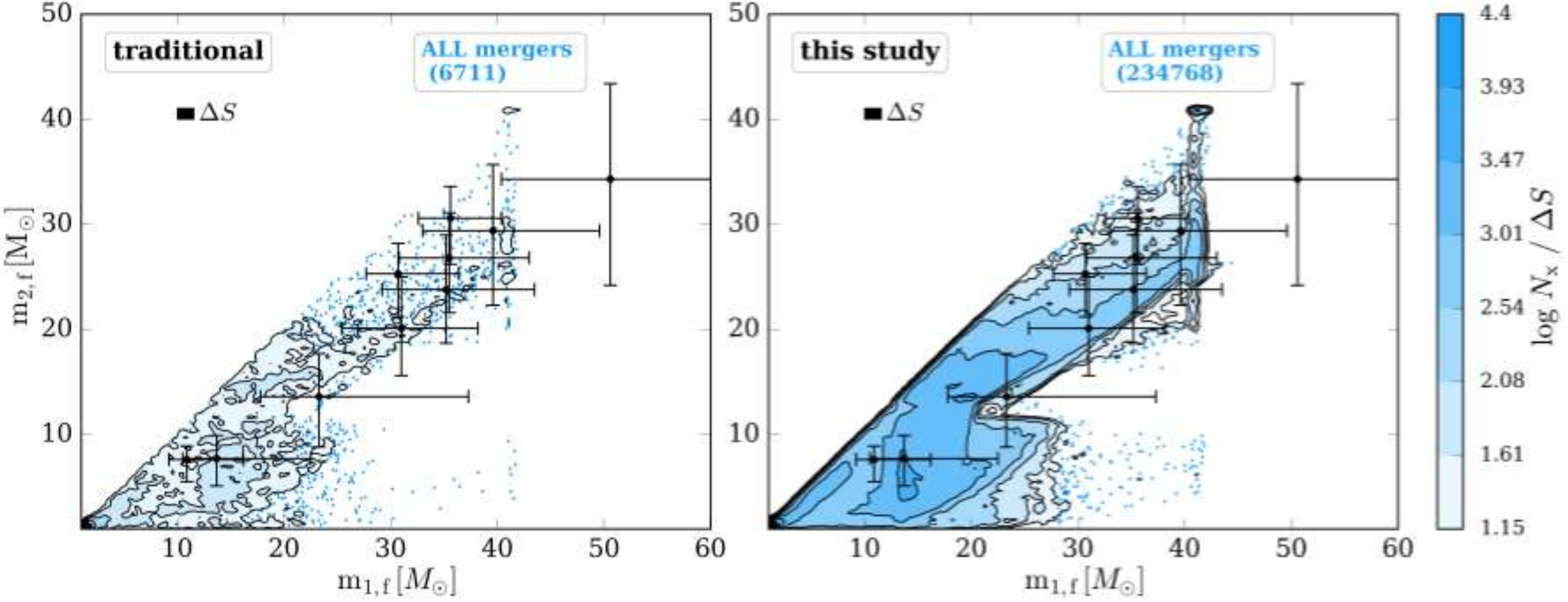
Higher resolution output



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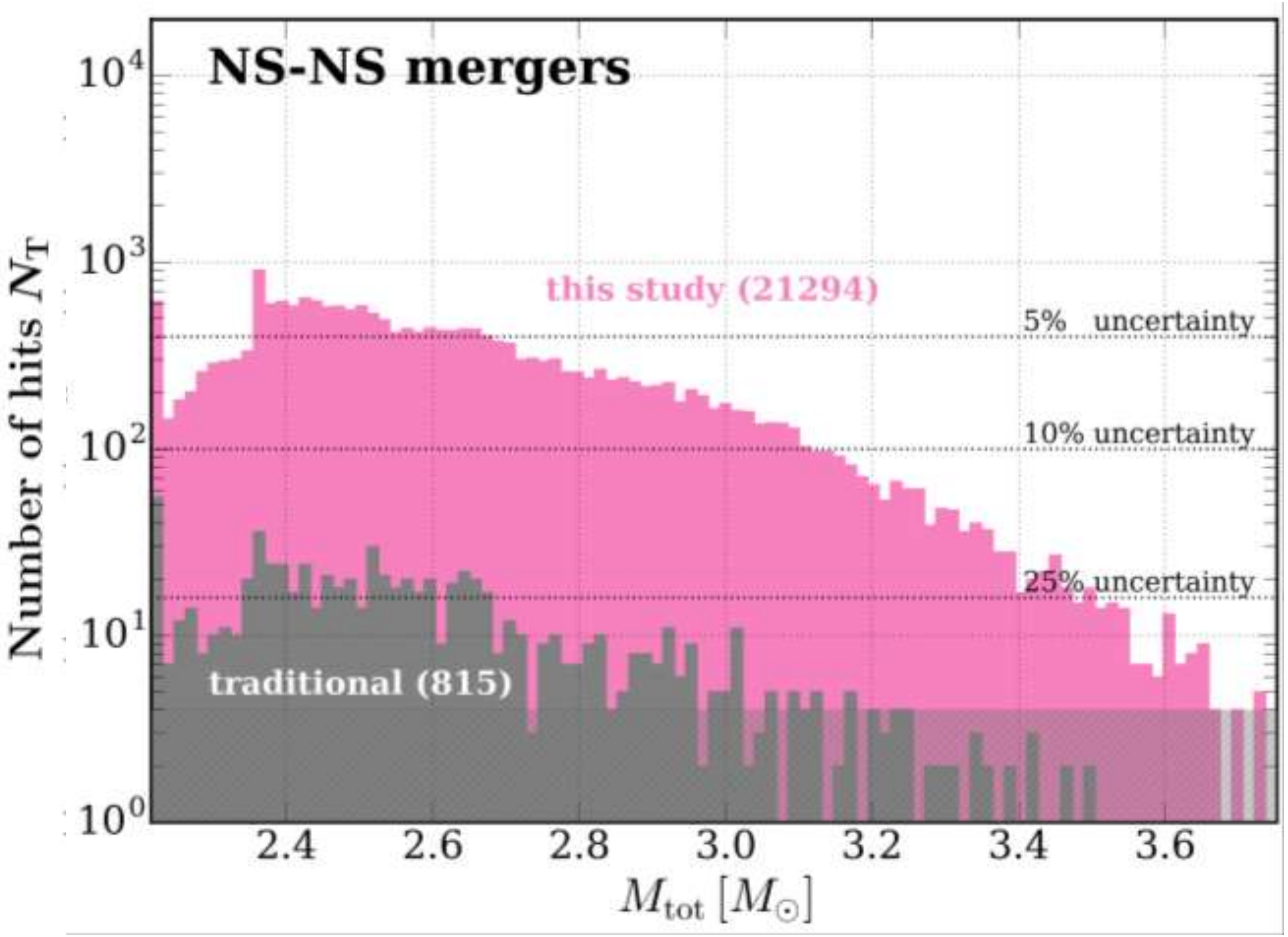
Resolve tails of distributions



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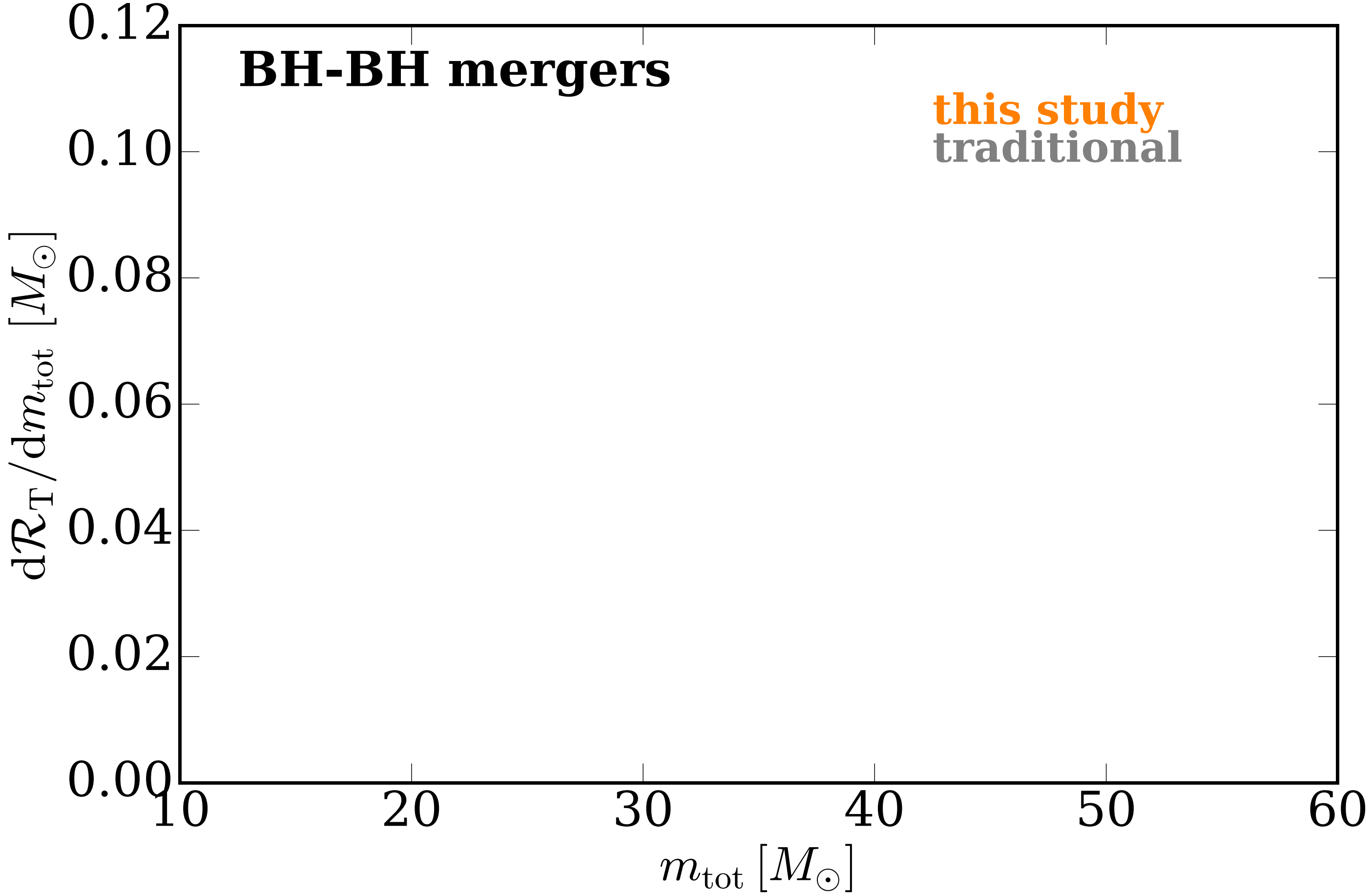
Better distribution functions



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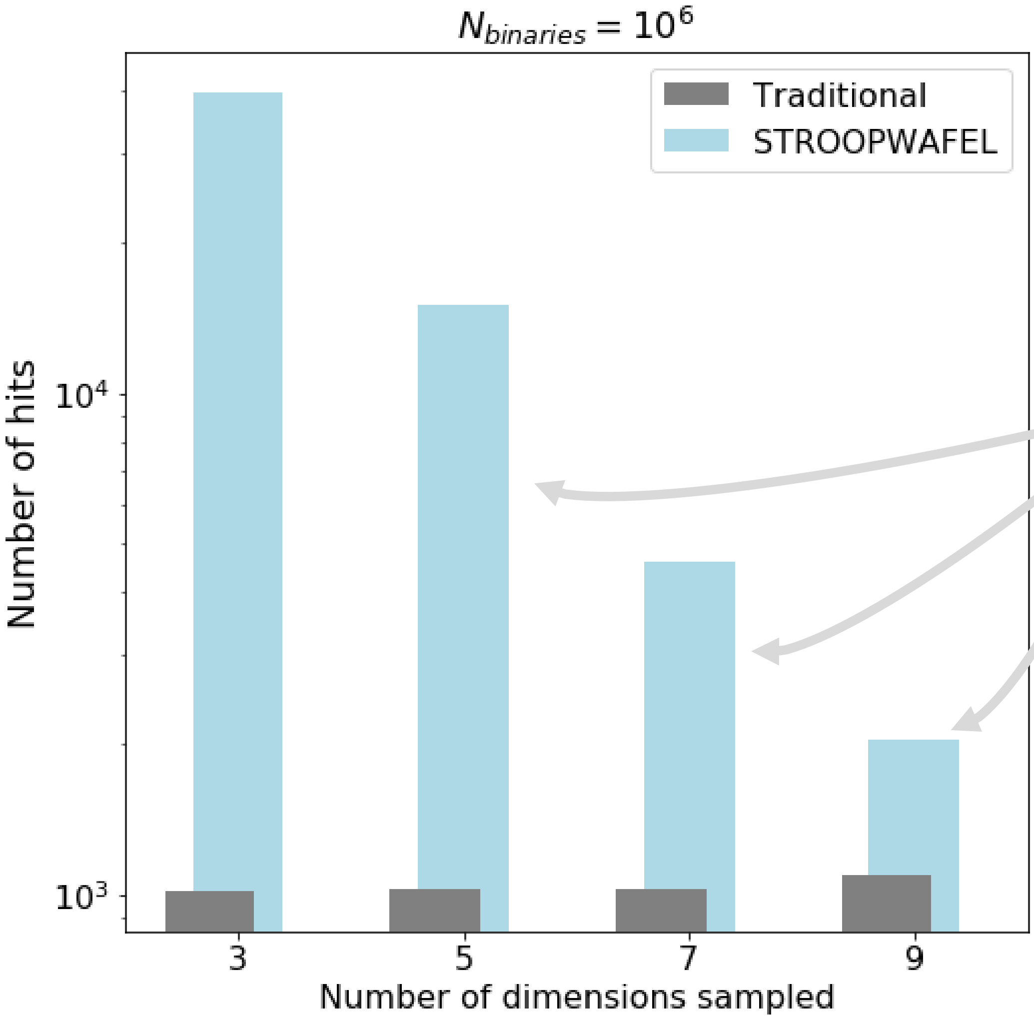
STROOPWAFEL paper accepted & public release of code & data:

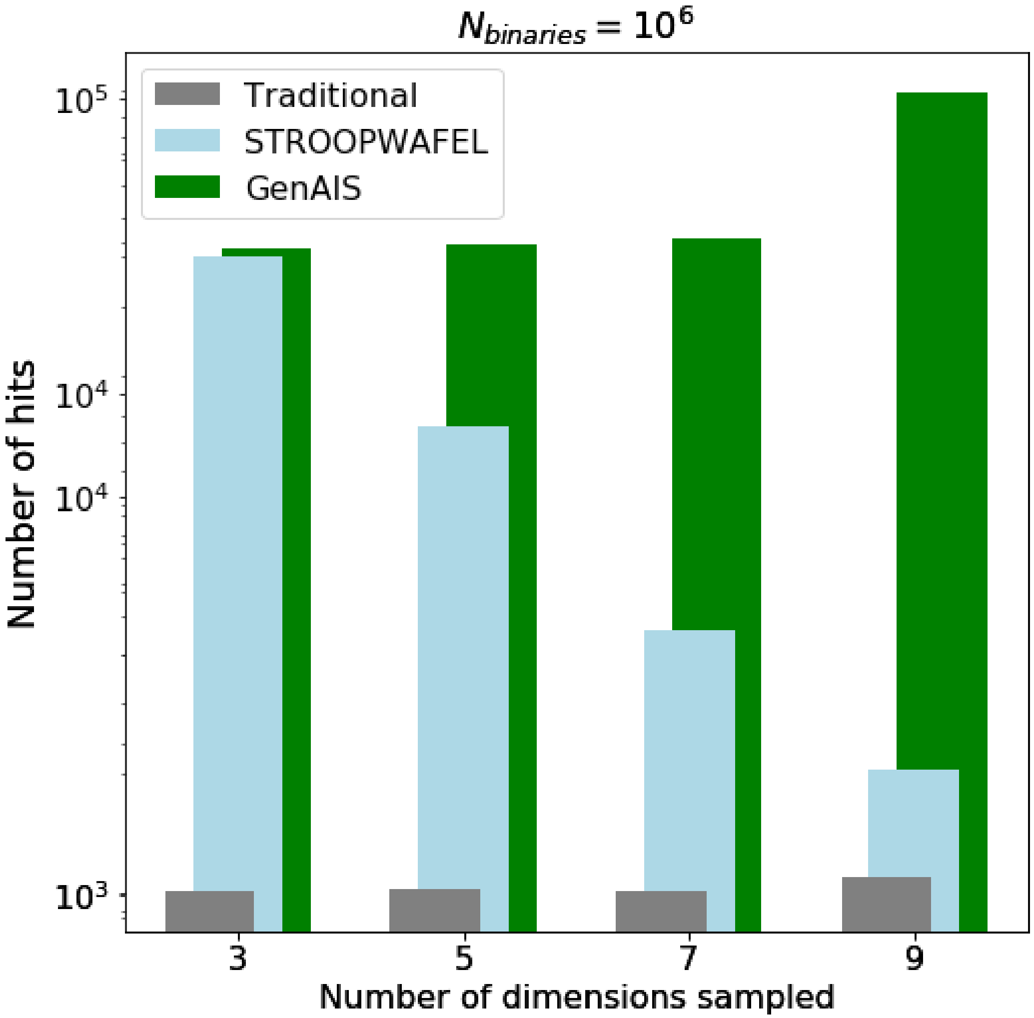


Higher dimensions?:

From Khandelwal in prep.

Curse of dimensionality suffered by STROOPWAFEL

Lokesh Khandelwal



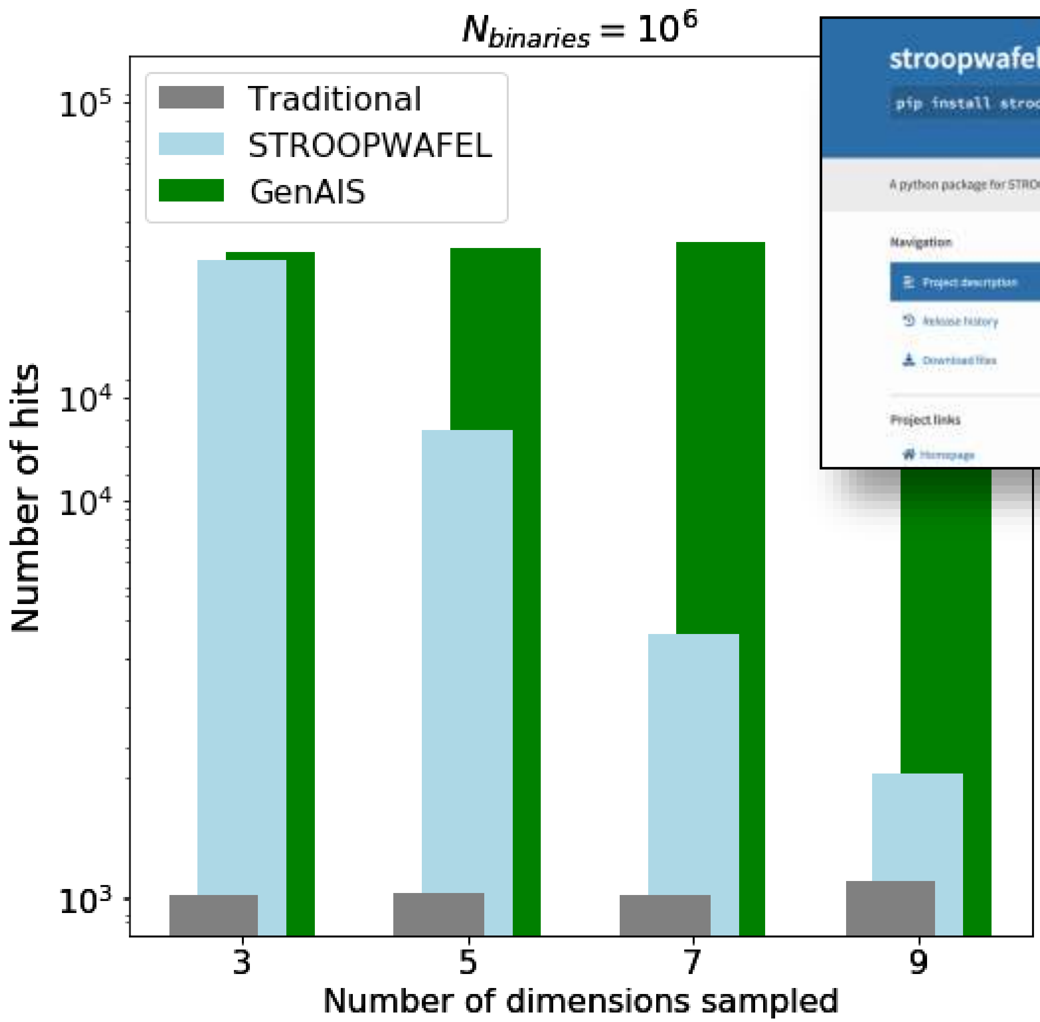
Higher dimensions?:

From Khandelwal in prep.

Curse of dimensionality suffered by STROOPWAFEL
improved using GenAIS (generational Adaptive Importance Sampling)
Based on Wraith+2009

Lokesh Khandelwal

Floor Broekgaarden



Based on Wraith+2009

Lokesh Khandelwal

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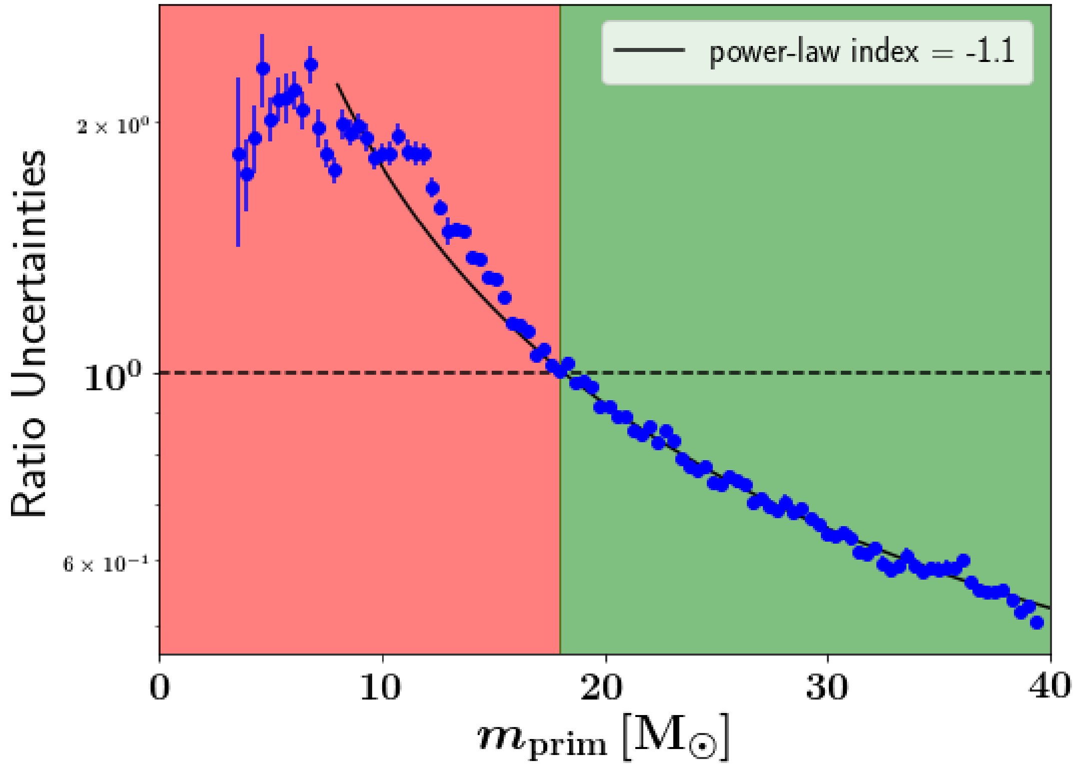
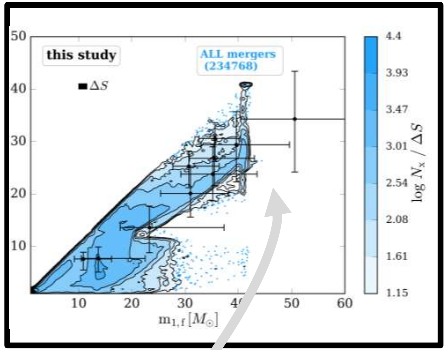
Observational selection biases?

Kummer et al. in prep.



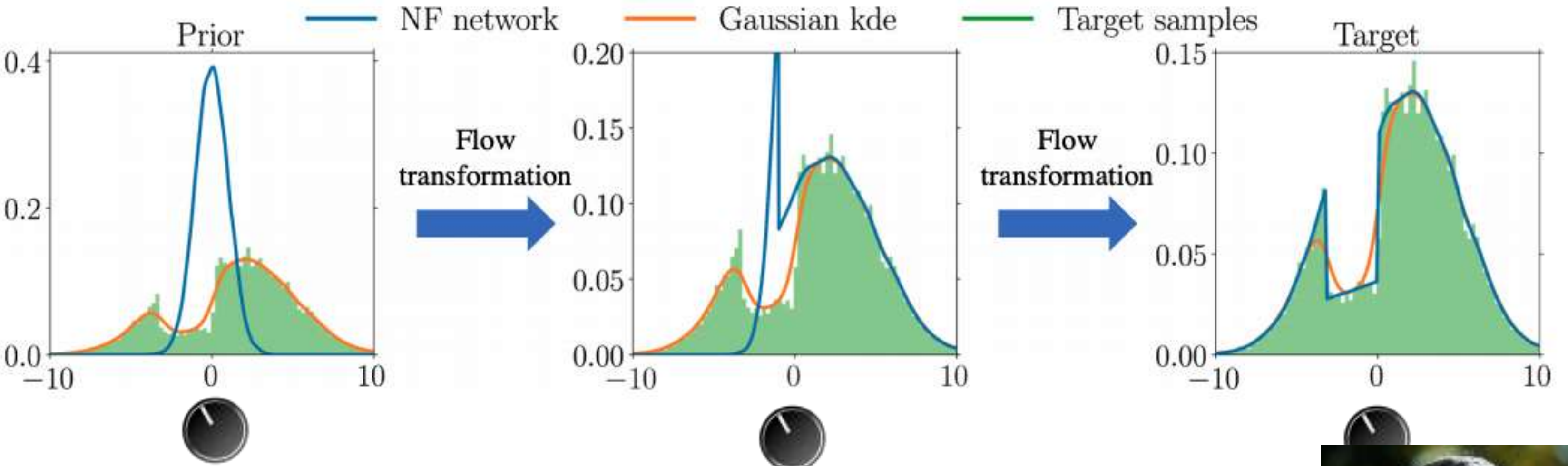


We want to improve resolution for the massive BH-BHs

Floris Kummer

Hierarchical Bayesian modeling with normalizing flows

ArXiv: 2002.09491
and 1909.06373

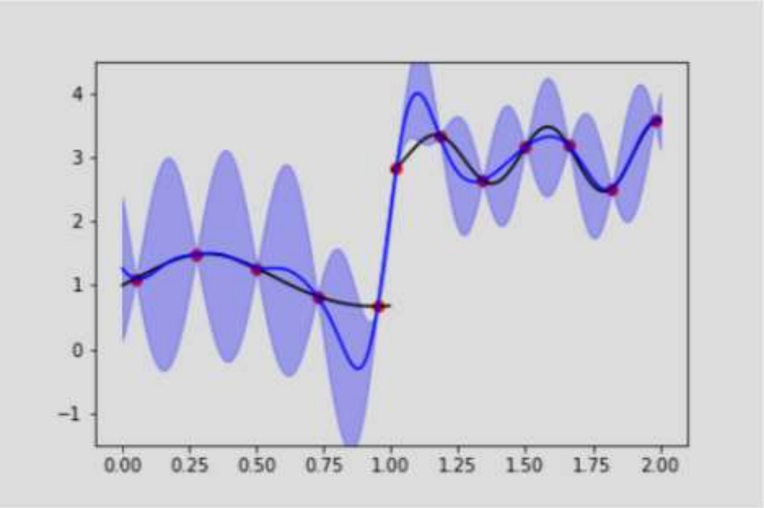


Kaze Wong
finishing PhD

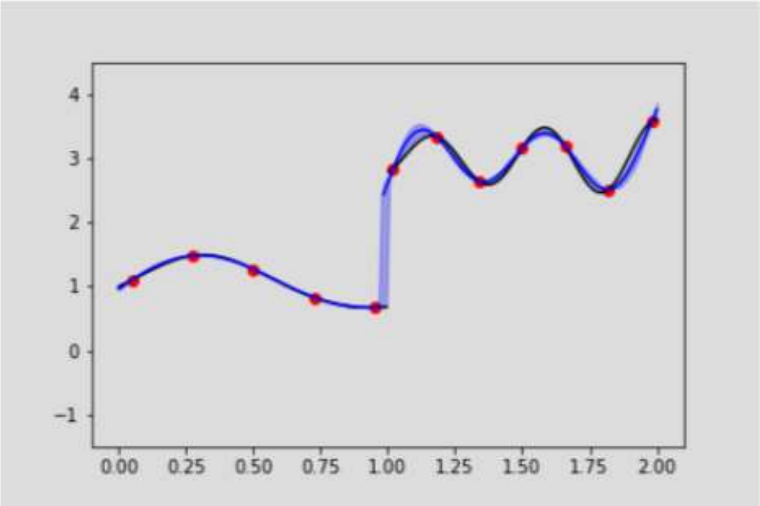
See also Kaze et al. recent work on using this for GWTC-2 in:
ArXiv: 2011.03564 and 2011.01865

Future work: Gaussian process classifiers & emulation + local response surface model

Traditional Gaussian Process Regression



Luyao Lin (in prep.)

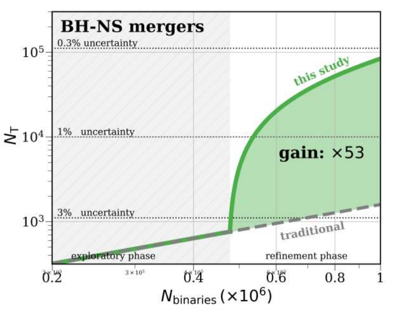


Luyao Lin

Derek Bingham

Floor Broekgaarden

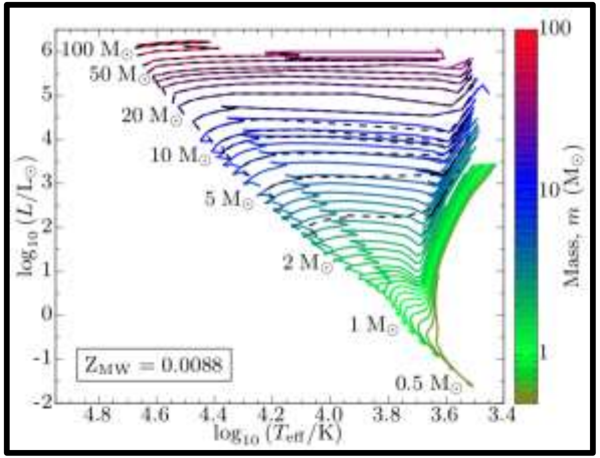
Conclusions

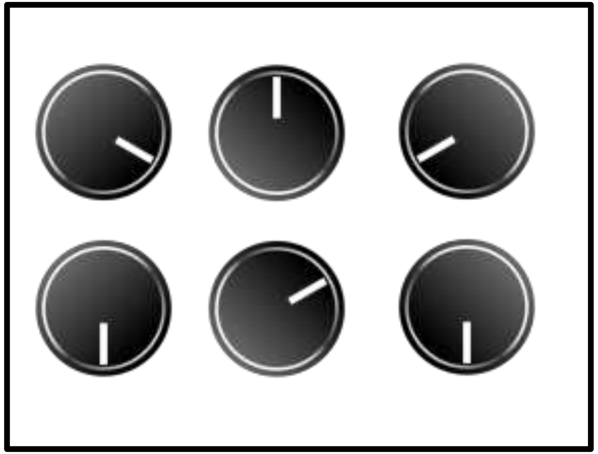


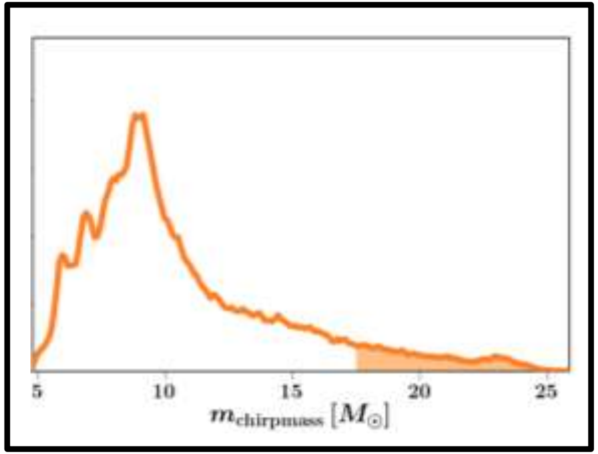
- STROOPWAFEL is an sampling algorithm that obtains $\times\, 30 - 200$ more hits or equivalently: speed up

Broekgaarden et al., 2019
Data, code and all scripts availa
 on Zenodo/github

STROOPWAFEL helps next generation simulations:







Include detailed prescriptions

Perform larger parameter study

Explore tails of distributions

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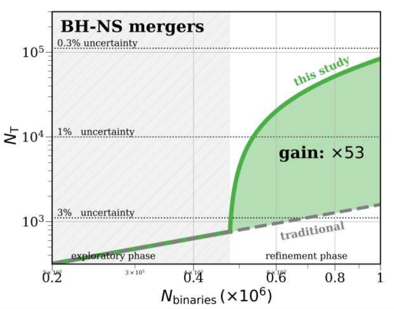
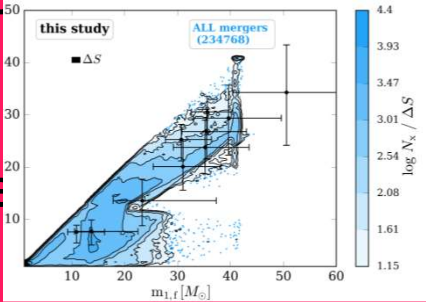
Conclusions



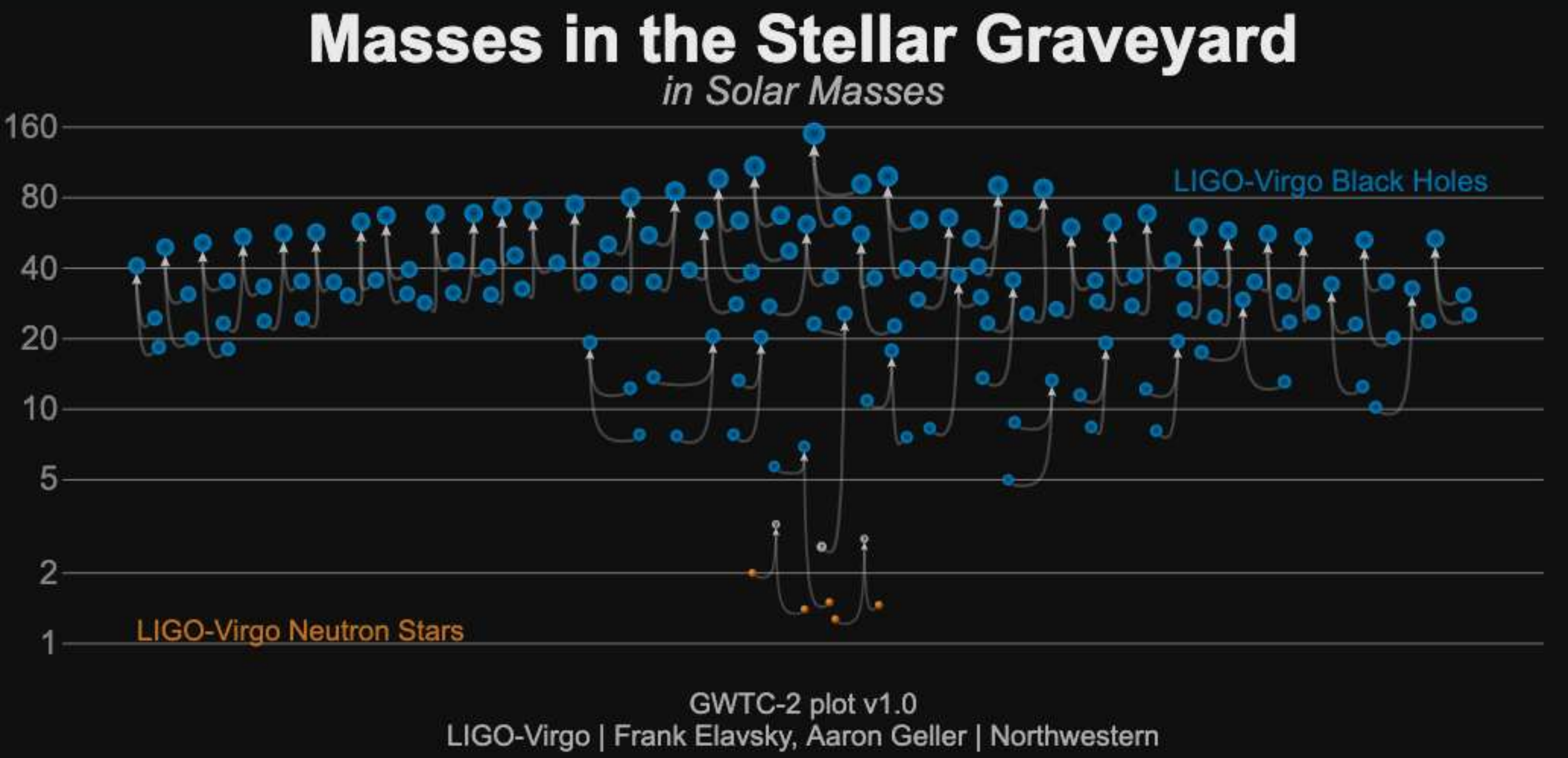
- STROOPWAFEL is an sampling algorithm that obtains $\times 30 - 200$ more hits or equivalently: speed up

- STROOPWAFEL improves resolution of population synthesis studies of GW events



- Future improvements are being actively developed + STROOPWAFEL is being implemented in other codes

Broekgaarden et al., 2019
Data, code and all scripts available on Zenodo/github



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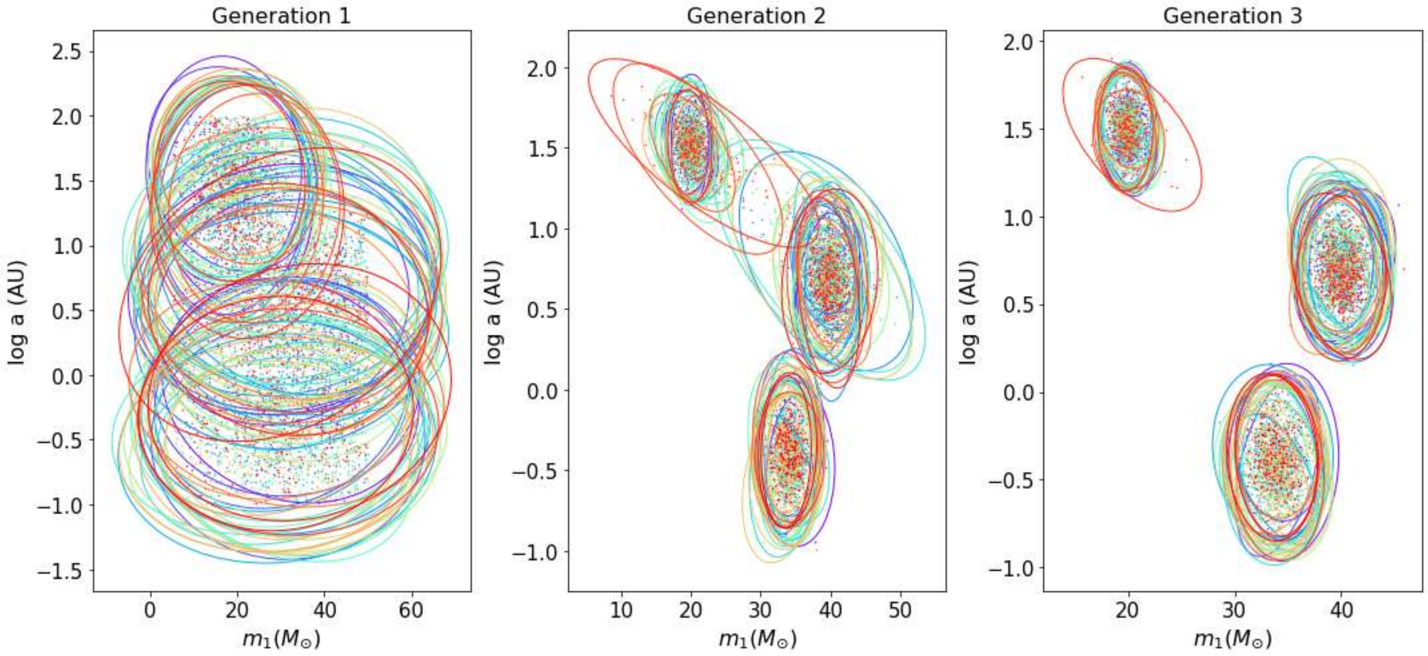
Thank you!

Image source: xkcd

Back-up slides

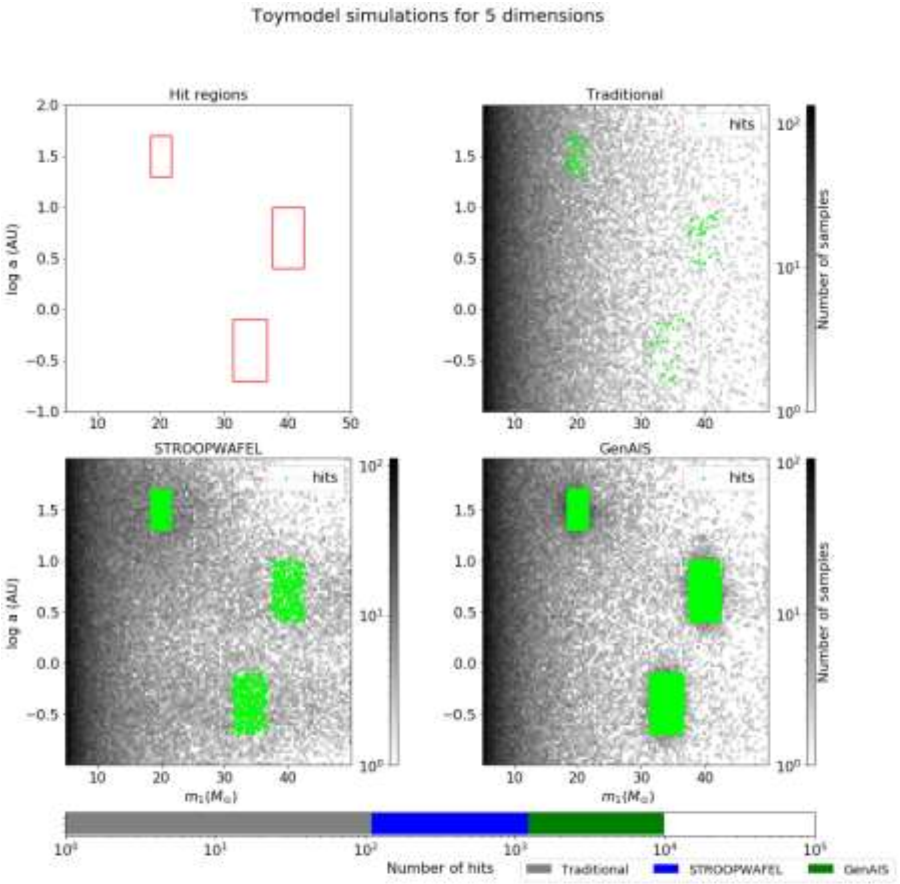
Future Prospects: more dimensions



Floris Kummer

Lokesh Khandelwal

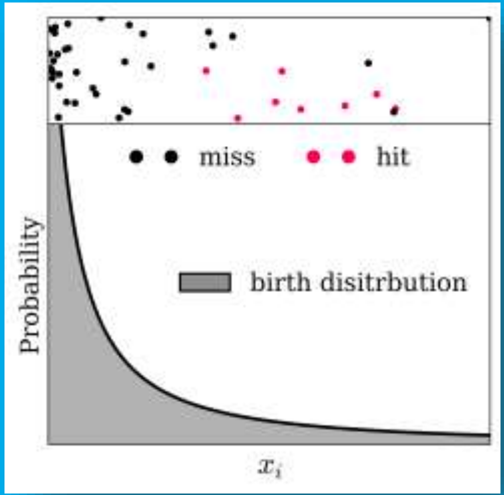
Future Prospects: more dimensions



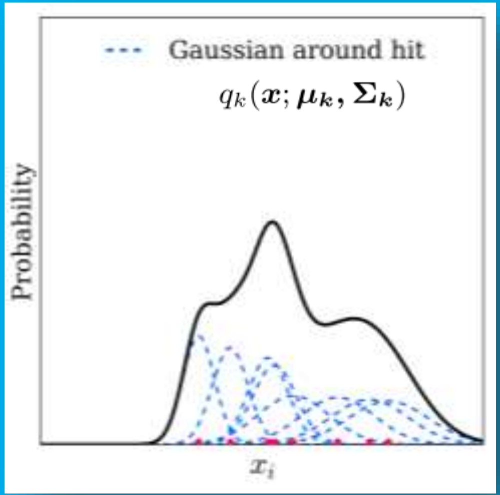
Floris Kummer

Lokesh Khandelwal

1) Exploring phase



2) Create adapted distribution



$$\boldsymbol{\Sigma_k} = \begin{bmatrix} \sigma_{1,k}^2 & 0 & \cdots \\ 0 & \ddots & \\ \vdots & & \sigma_{d,k}^2 \end{bmatrix},$$

$$\sigma_{j,k} = \kappa \frac{1}{\pi_j(x_k) N_{\mathrm{expl}}^{1/d}},$$

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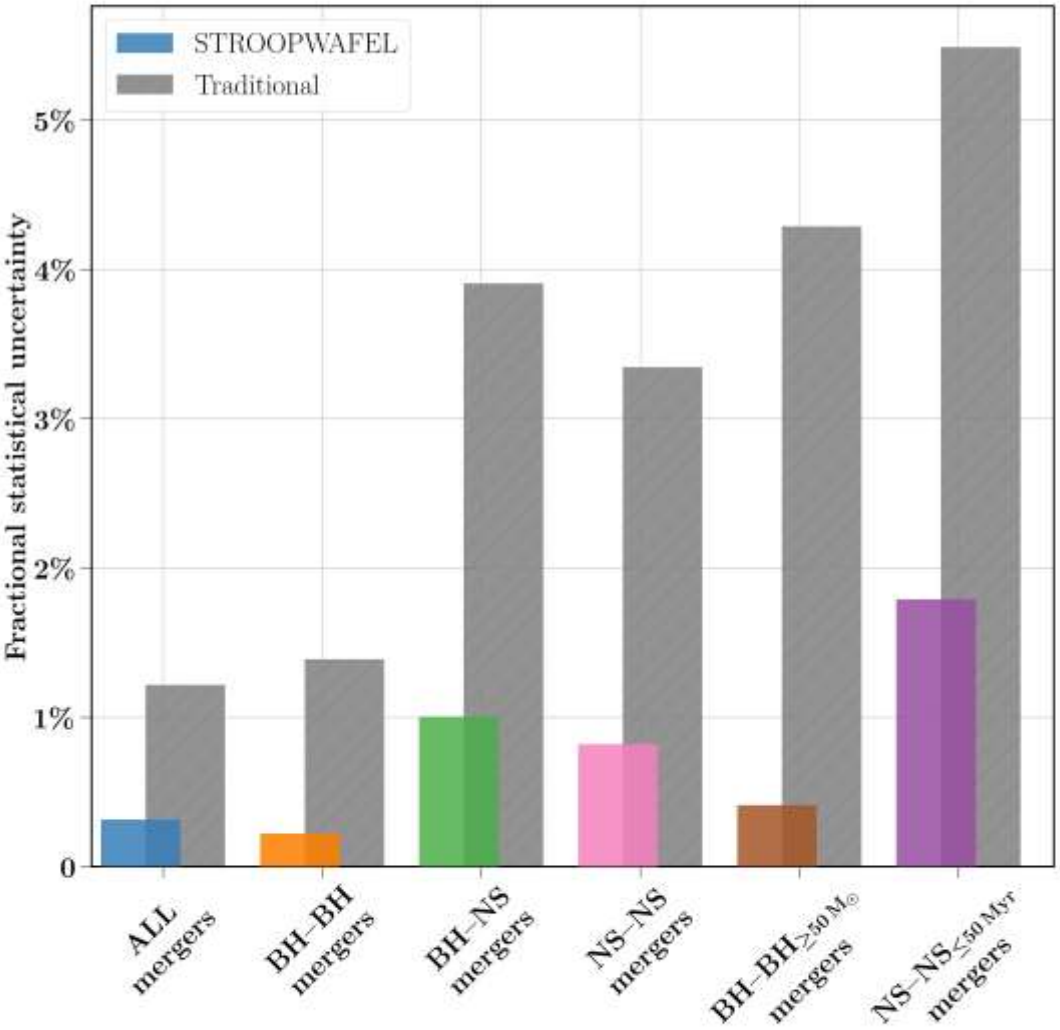

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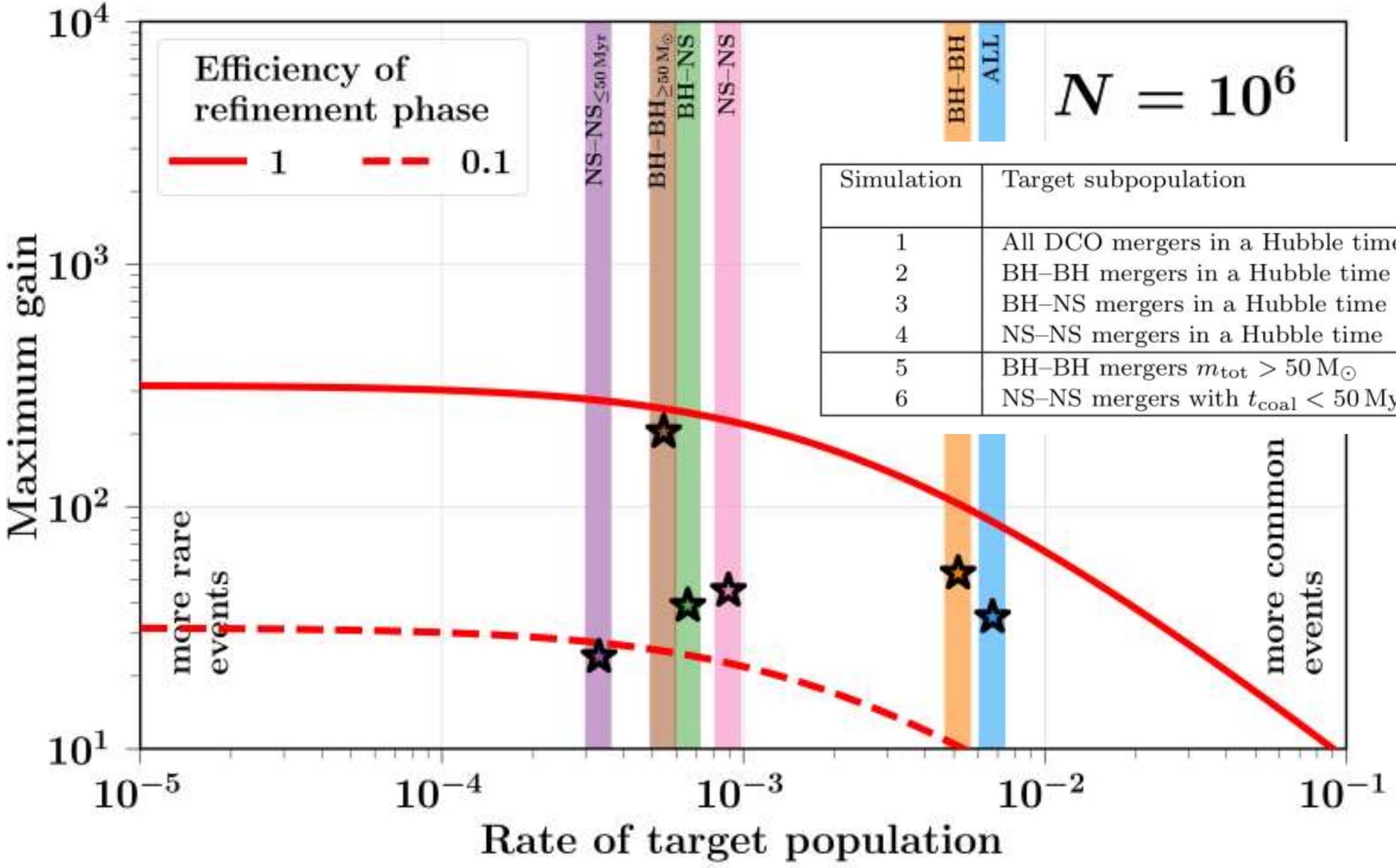

Simulation	Target subpopulation	gain
1	All DCO mergers in a Hubble time	35×
2	BH–BH mergers in a Hubble time	53×
3	BH–NS mergers in a Hubble time	39×
4	NS–NS mergers in a Hubble time	45×
5	BH–BH mergers $m_{\mathrm{tot}} > 50\,\mathrm{M}_\odot$	202×
6	NS–NS mergers with $t_{\mathrm{coal}} < 50\,\mathrm{Myrs}$	24×

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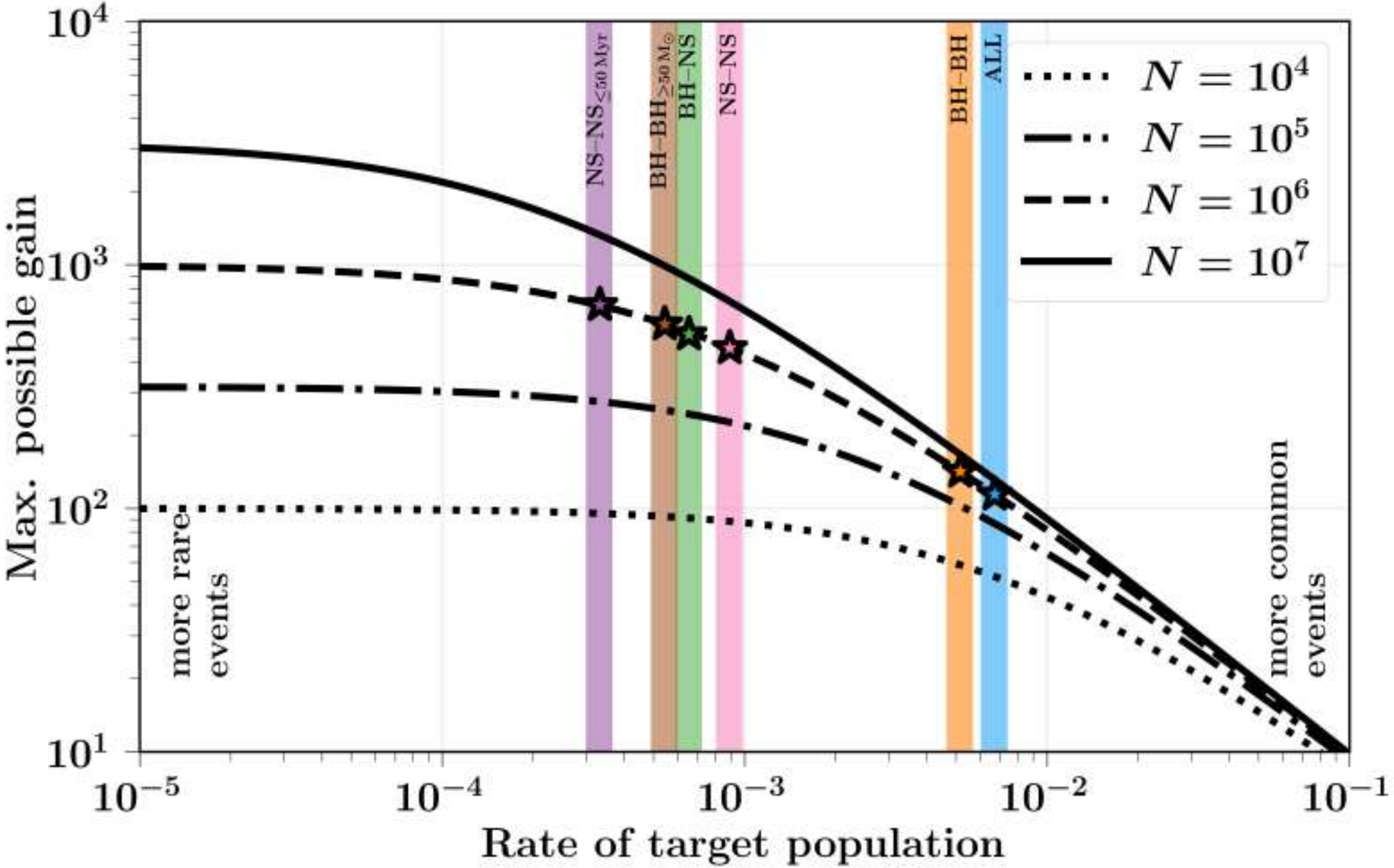
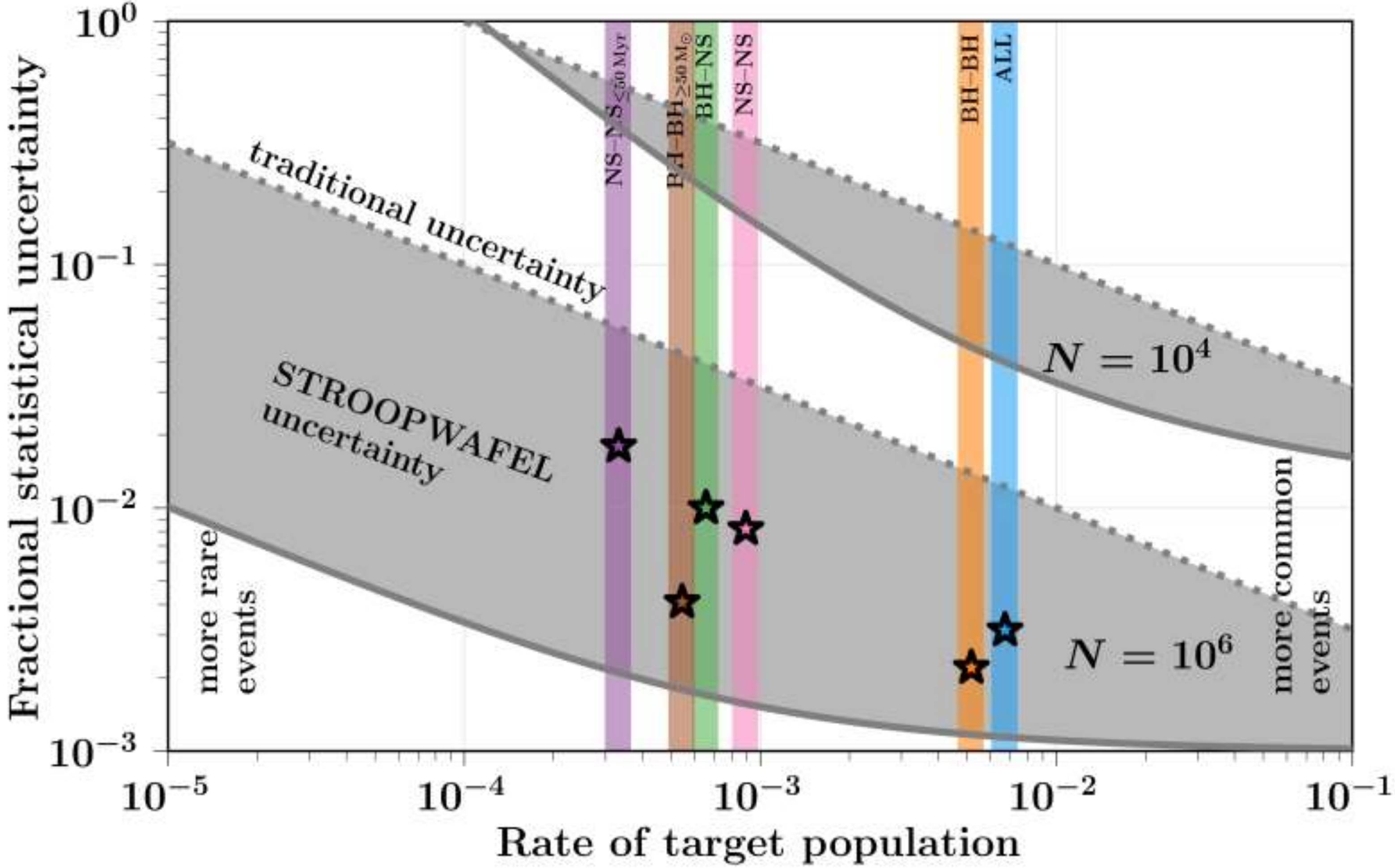
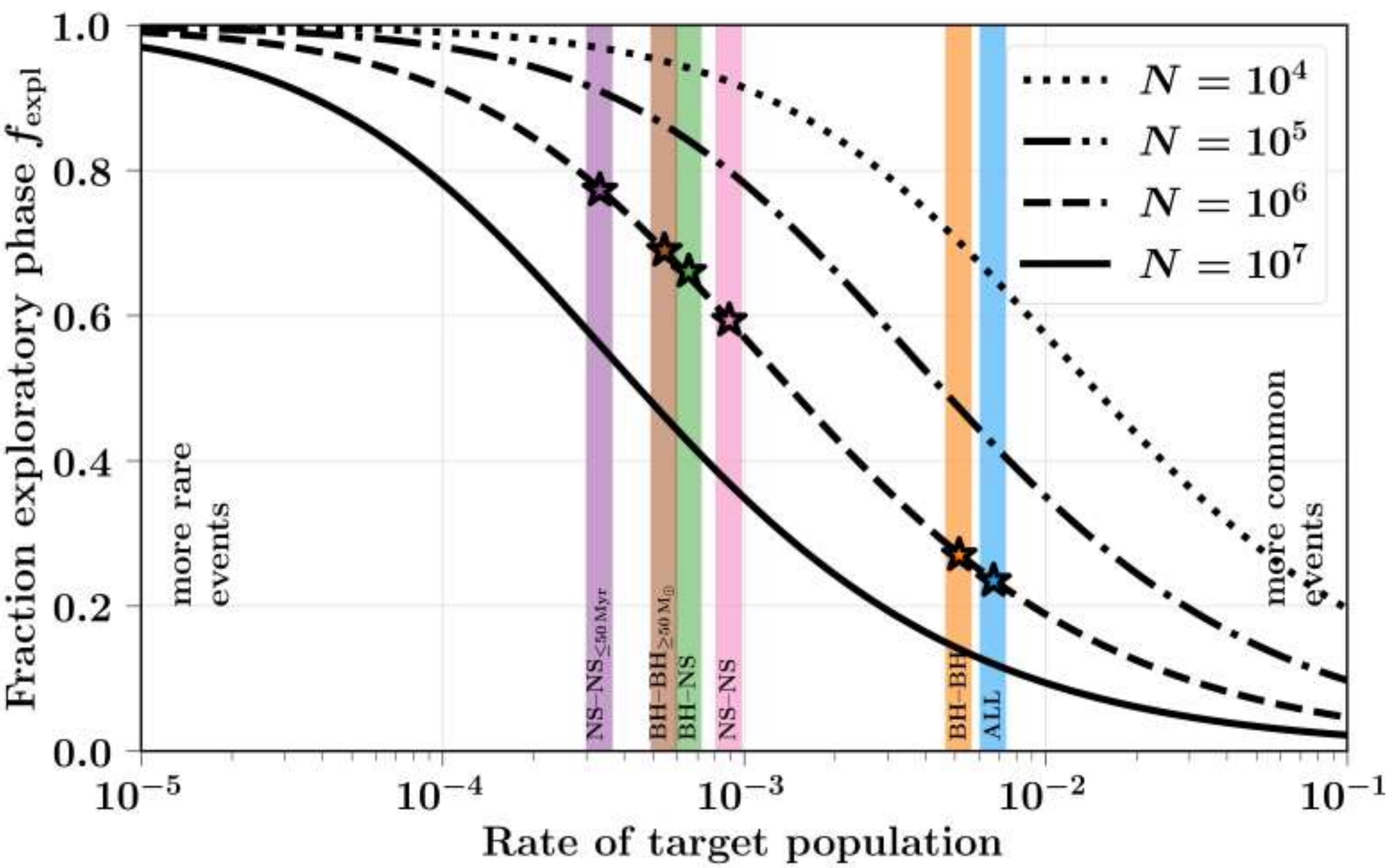


Floor Broekgaarden

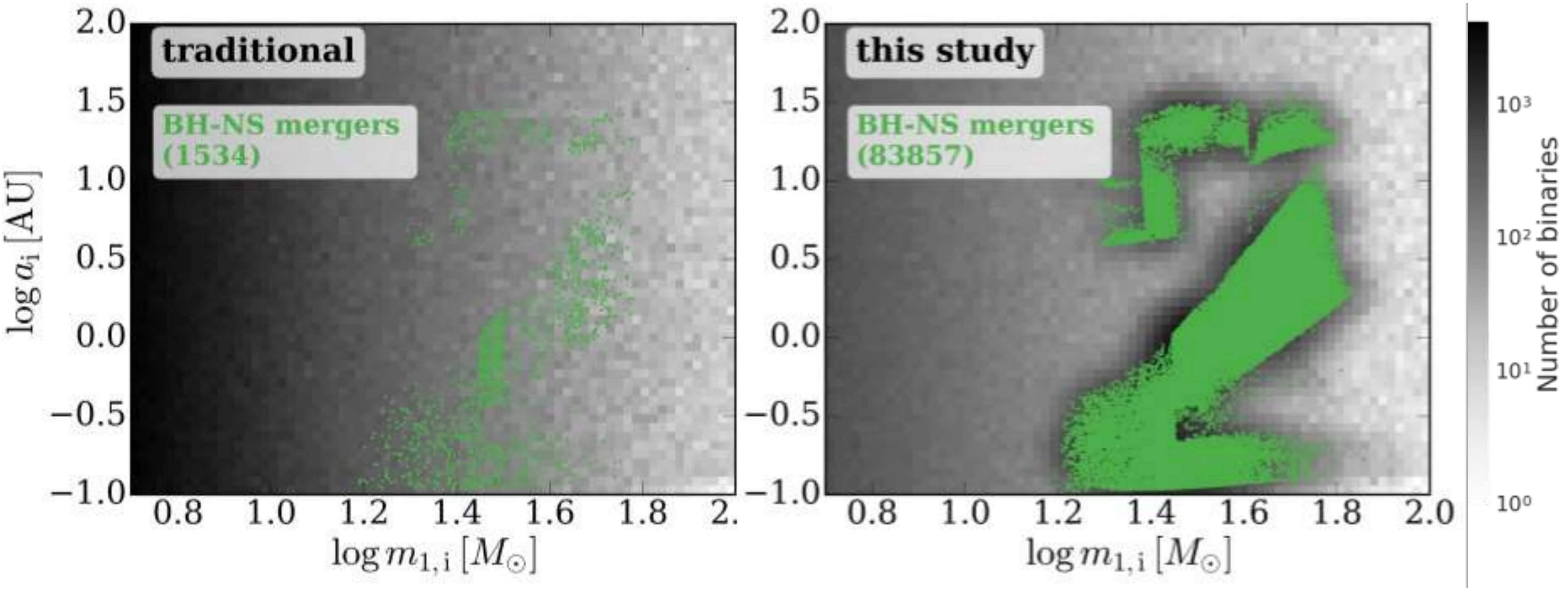


Floor Broekgaarden



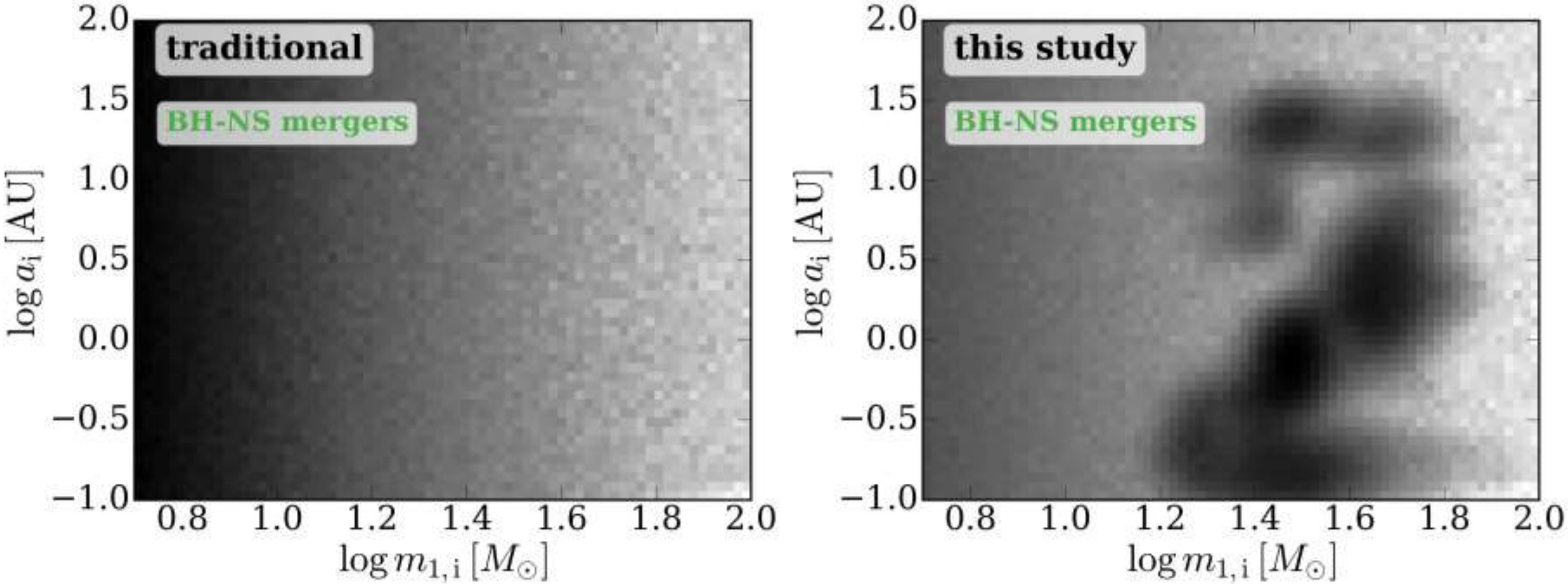
Floor Broekgaarden

Better resolution progenitors

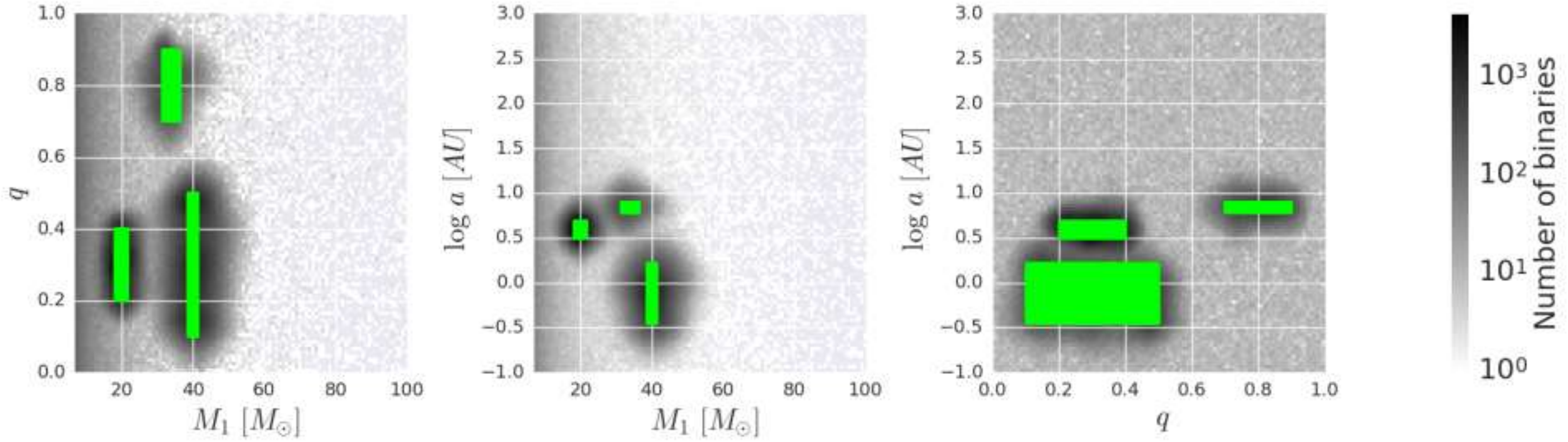


Floor Broekgaarden

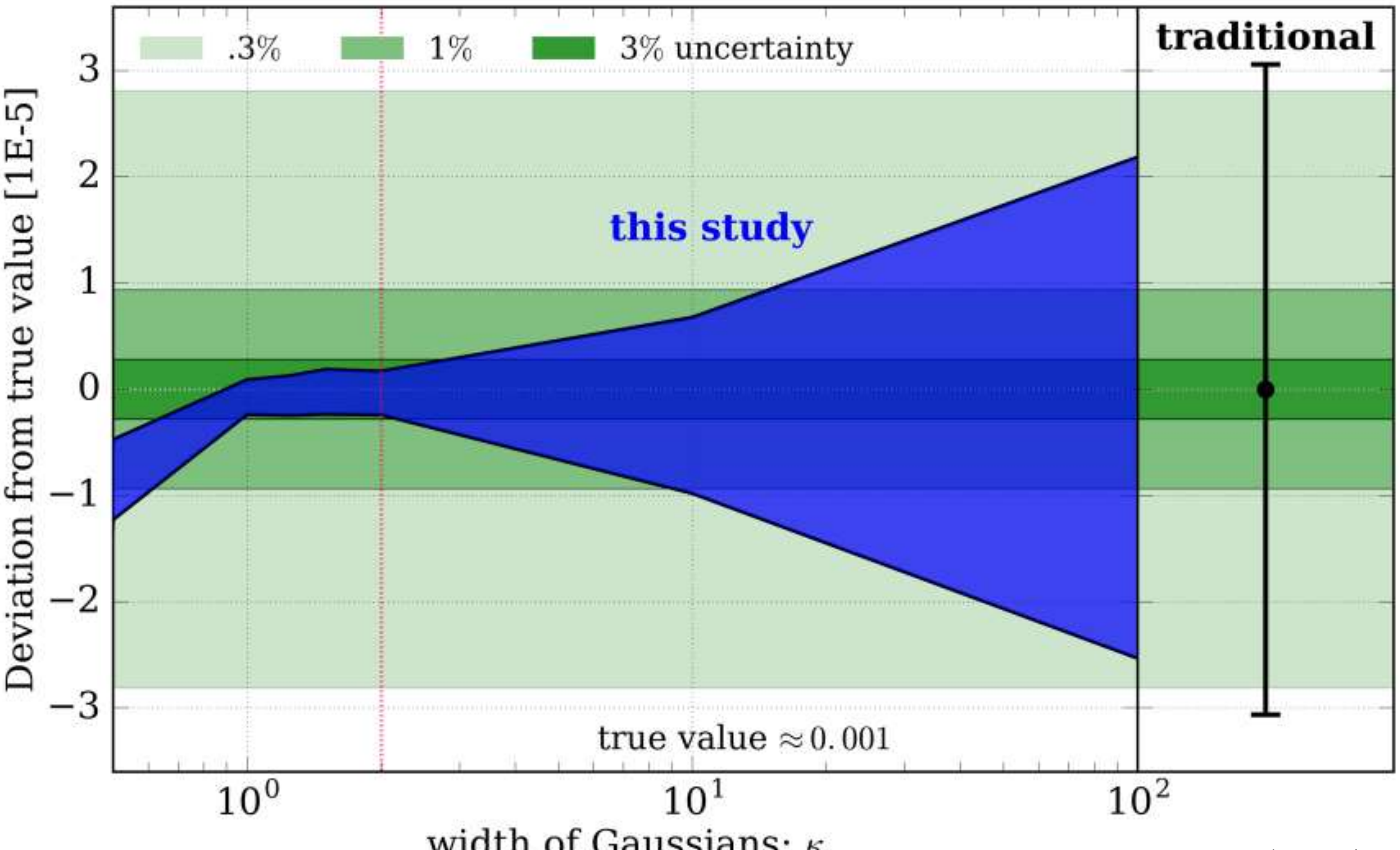
Refinement phase



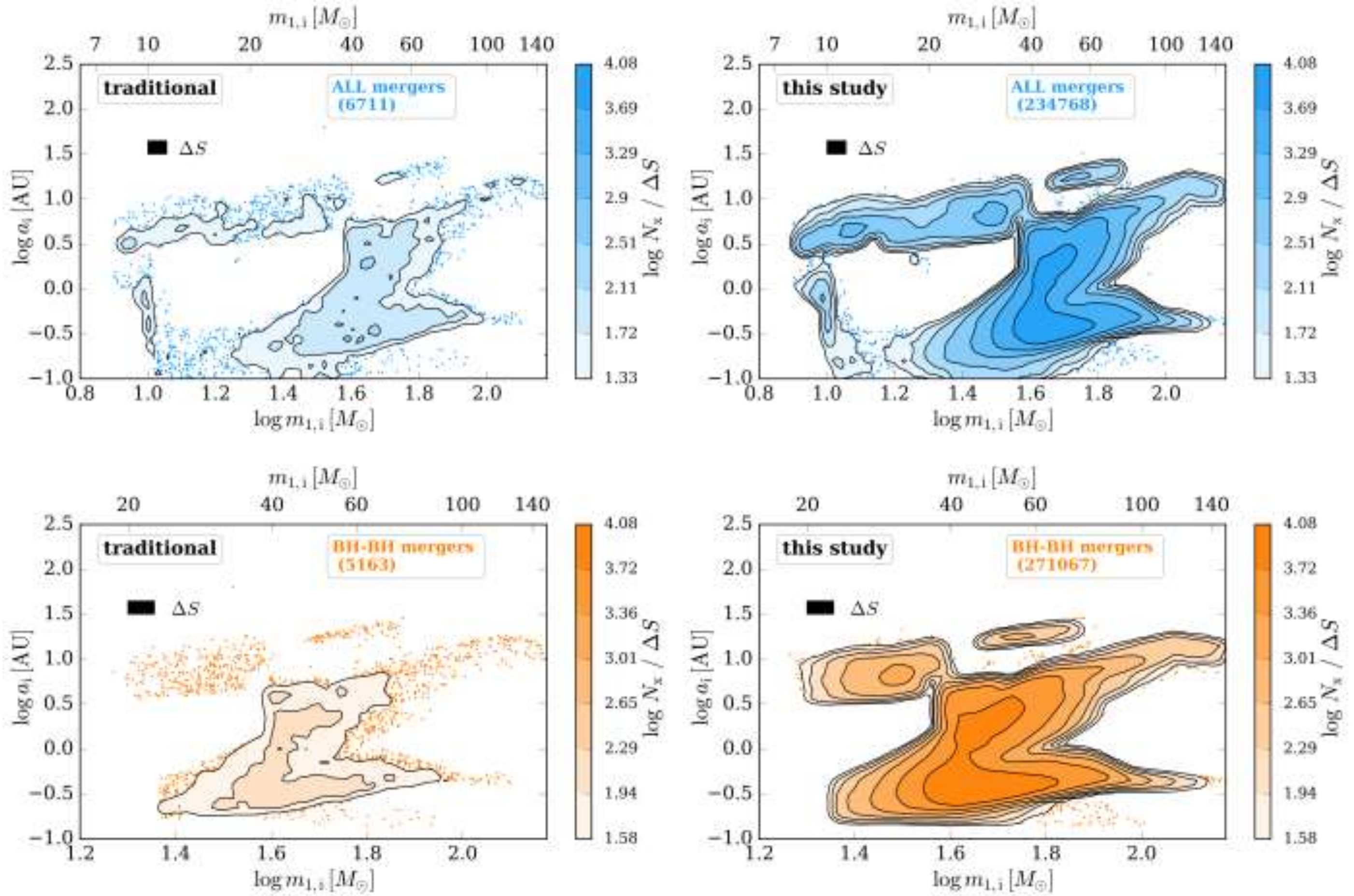
Floor Broekgaarden



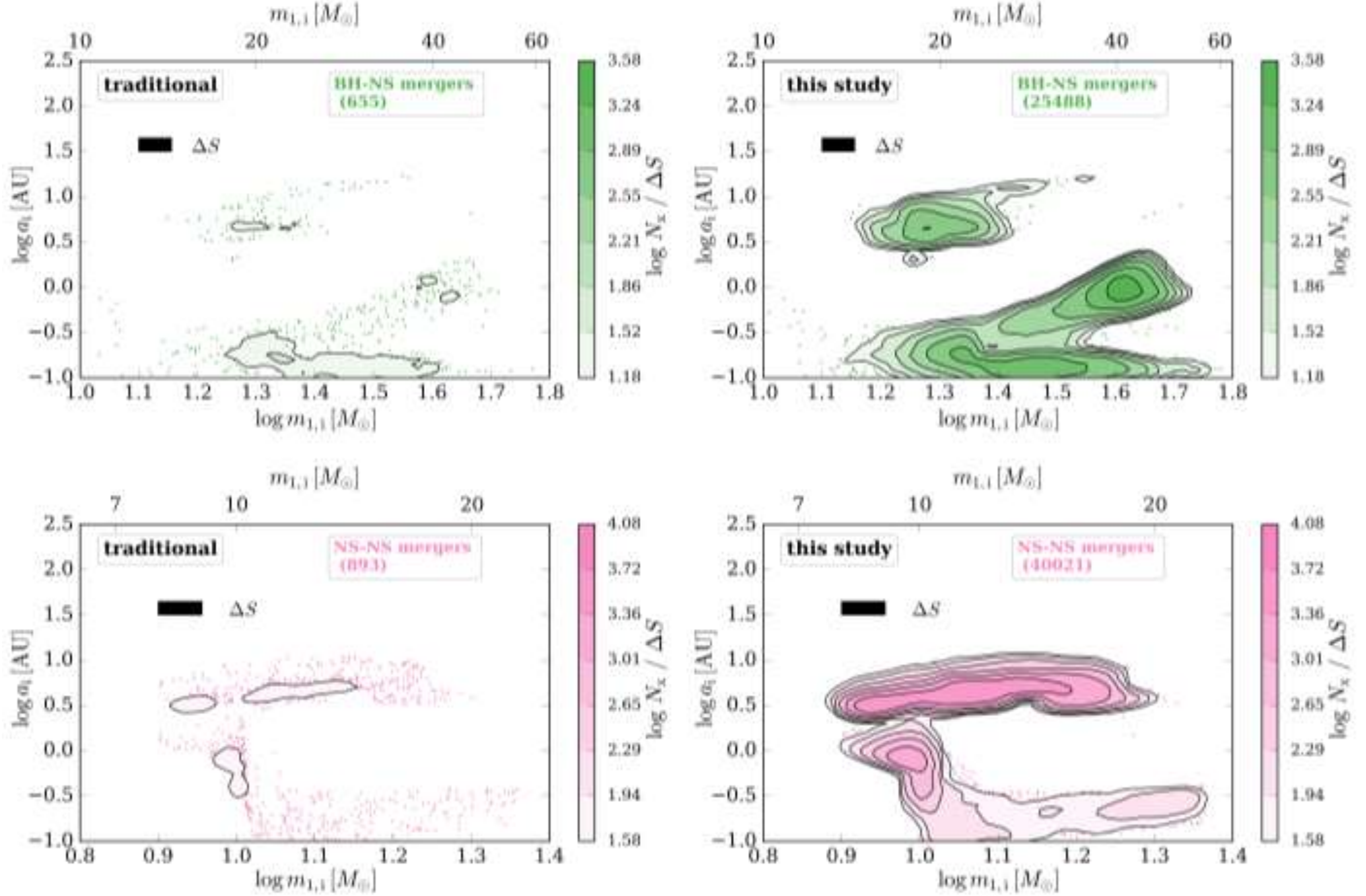
Floor Broekgaarden



Floor Broekgaarden



Floor Broekgaarden



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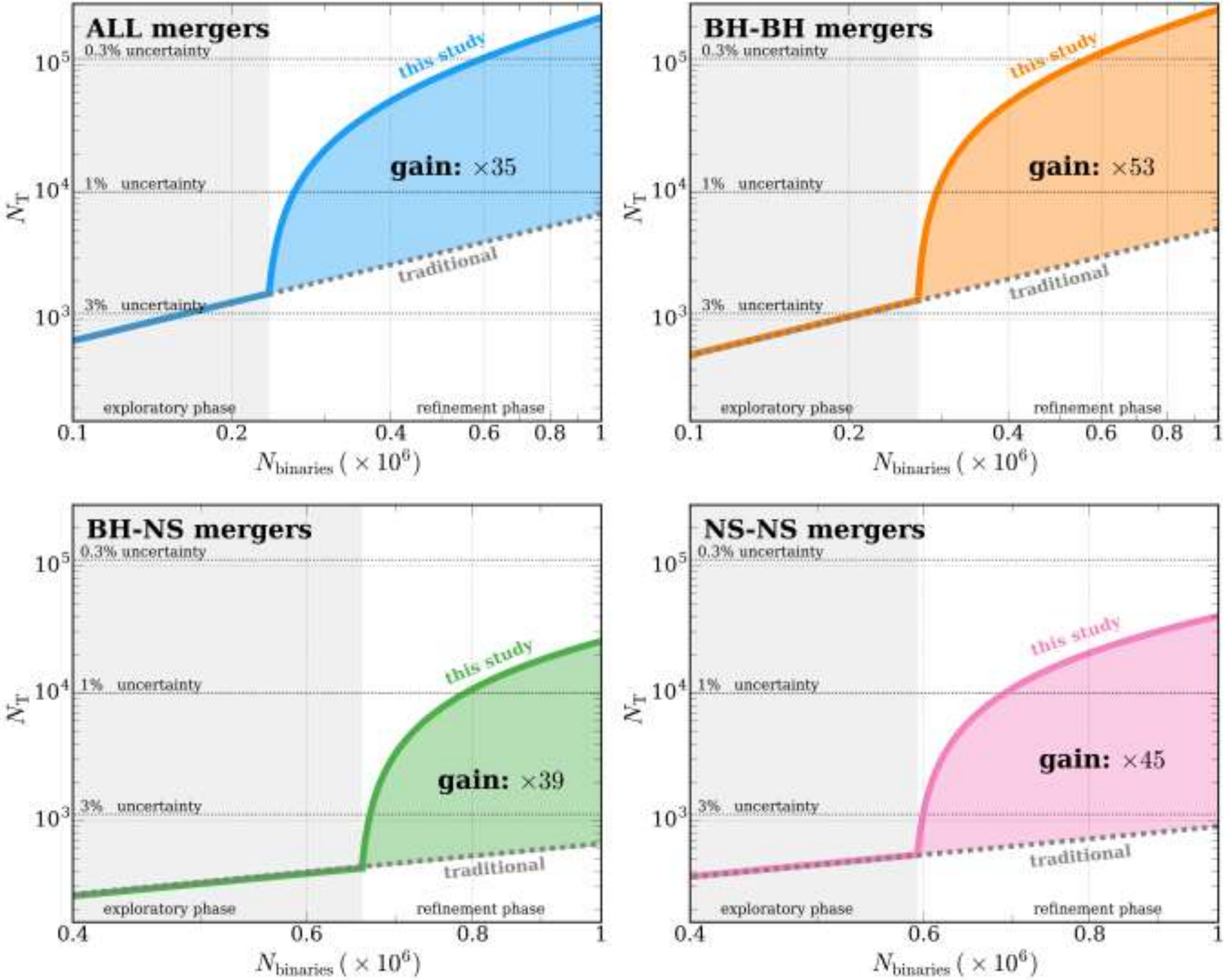
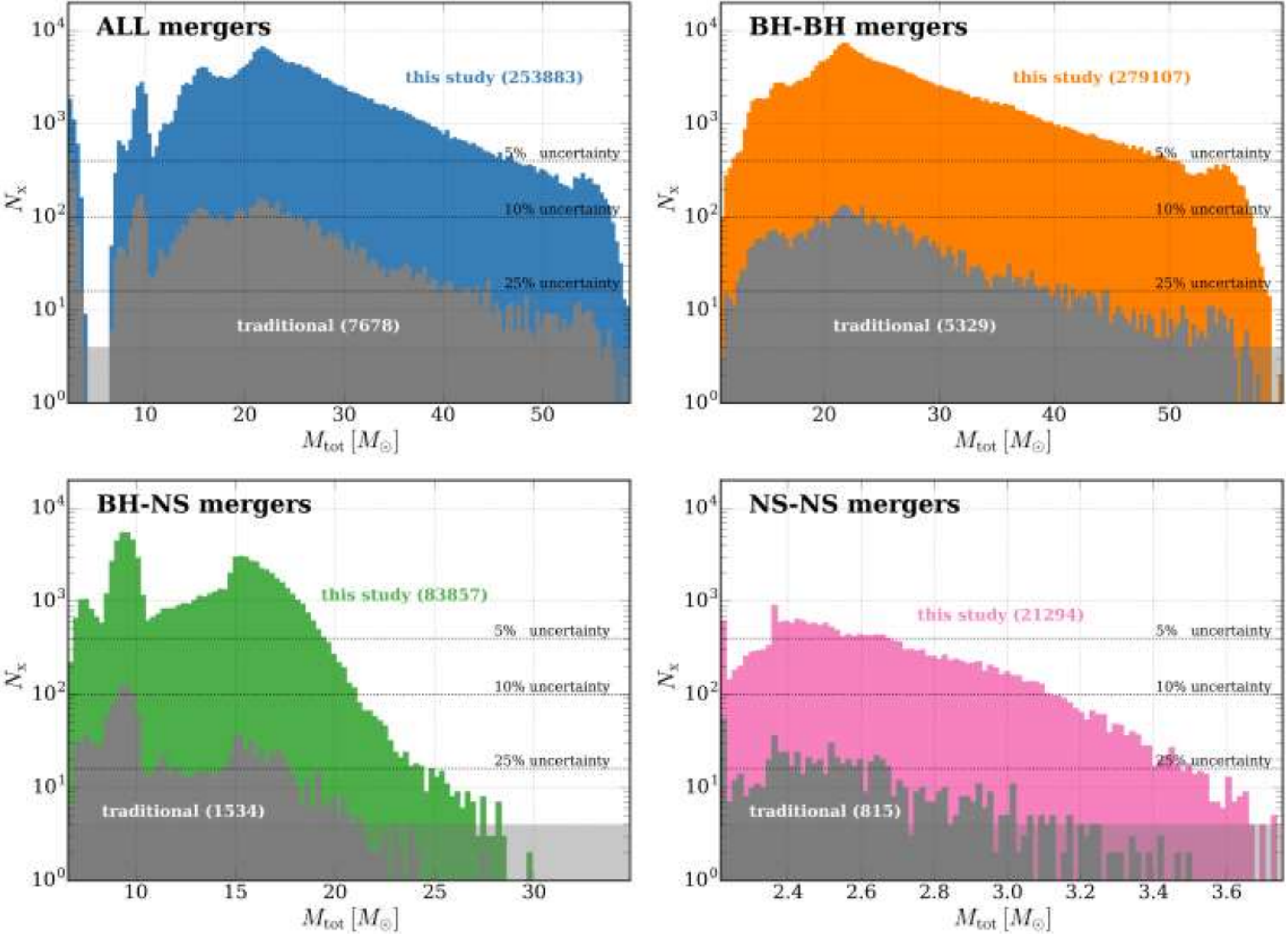
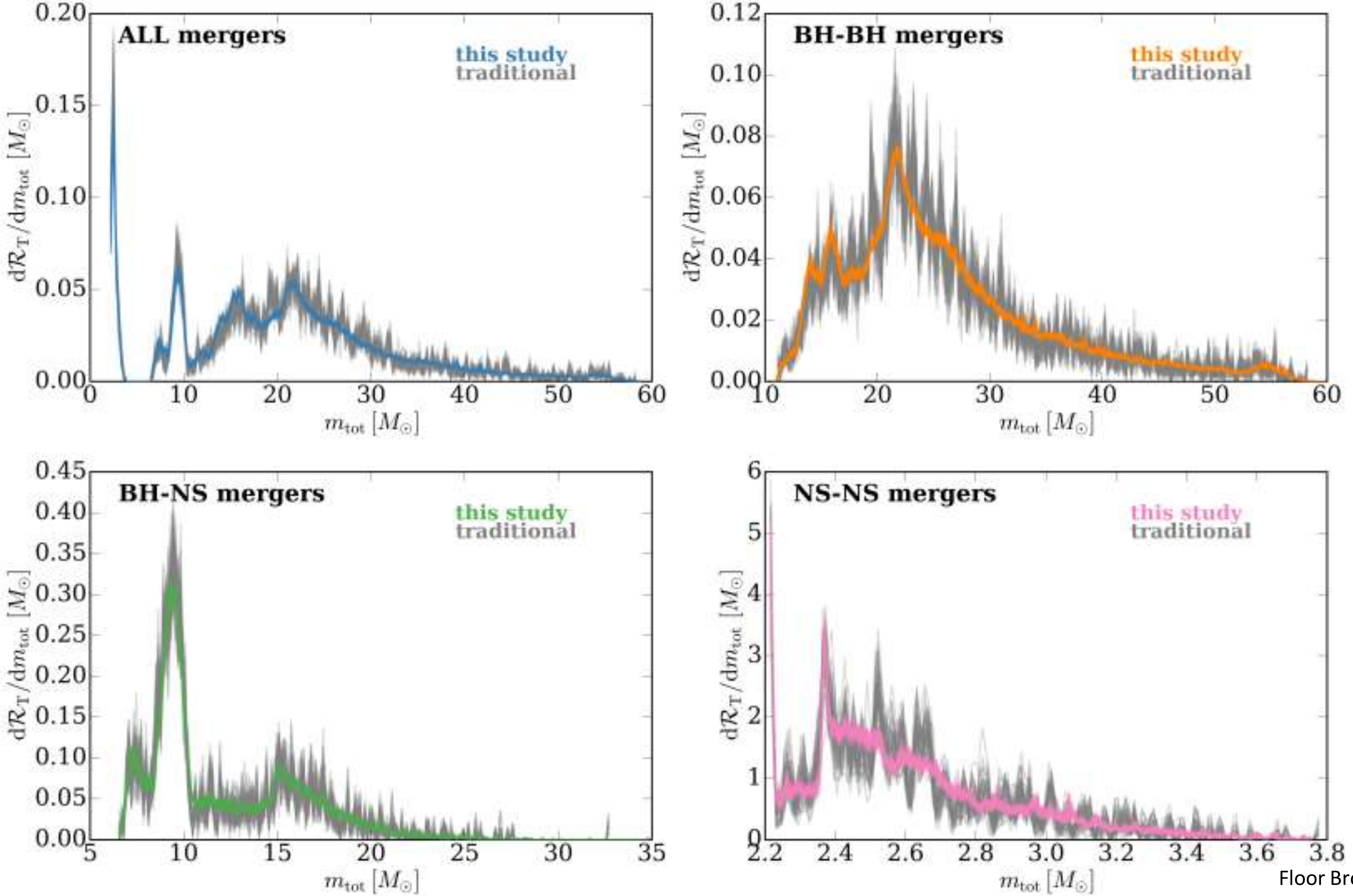


ALL mergers
BH-BH mergers
BH-NS mergers
NS-NS mergers
0.3% uncertainty
1% uncertainty
3% uncertainty
this study
traditional
gain: ×35
gain: ×53
gain: ×39
gain: ×45
exploratory phase
refinement phase
N_{T}
$N_{\mathrm{binaries}}\ (\times 10^6)$



Floor Broekgaarden



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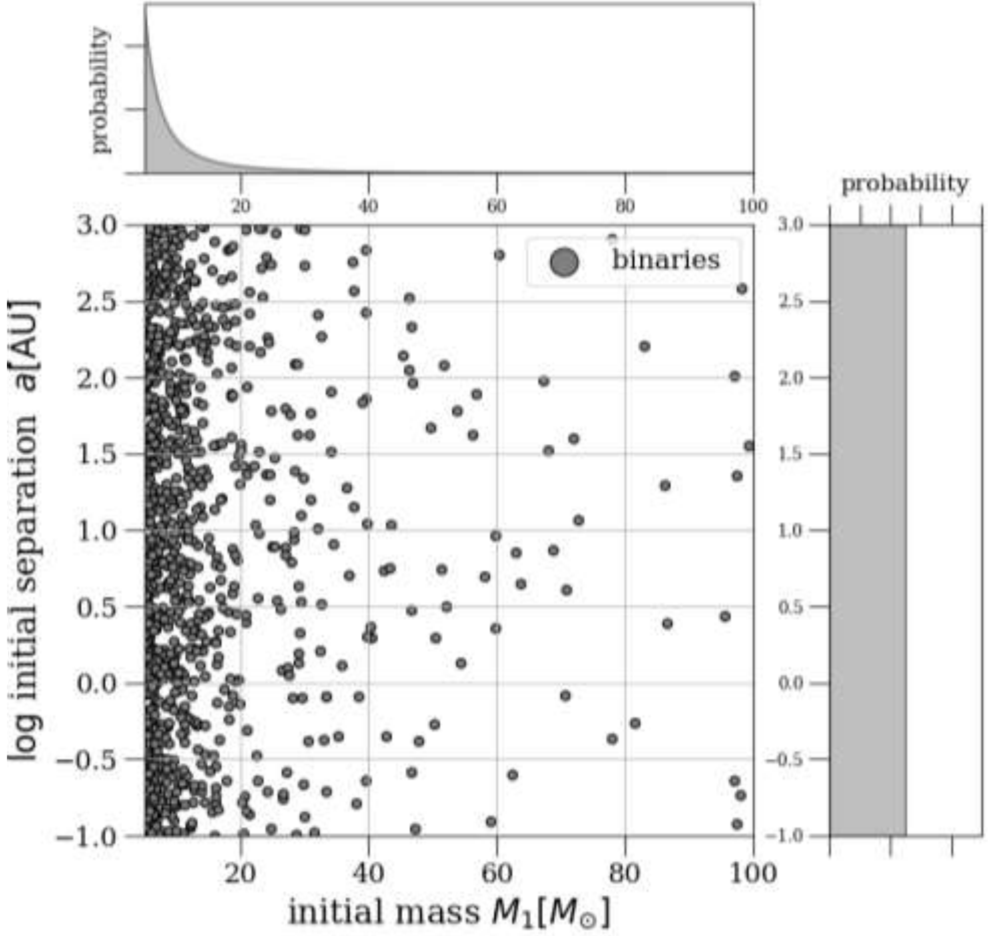
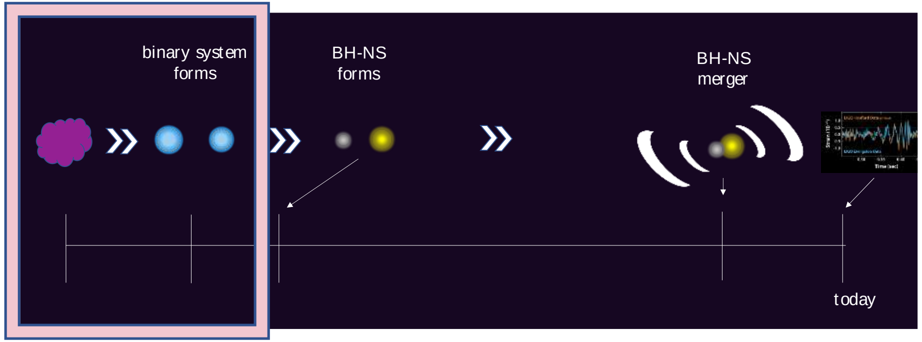
1 Populations:



E.g. Belczynski+02

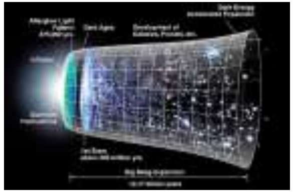
Two processes impact the predicted gravitational wave observations:

1. Star formation history over cosmic time?



Describes "model for the Universe":

$$\mathrm{MSSFR}(z_{\mathrm{form}}) = \underbrace{\frac{d^2 M_{\mathrm{SFR}}}{dt_s dV_c}(z_{\mathrm{form}})} \times \underbrace{\frac{dM_{\mathrm{SFR}}}{dZ}(z_{\mathrm{form}})},$$



Star formation rate **SFR(z)**

Chemical evolution **Z(z)**

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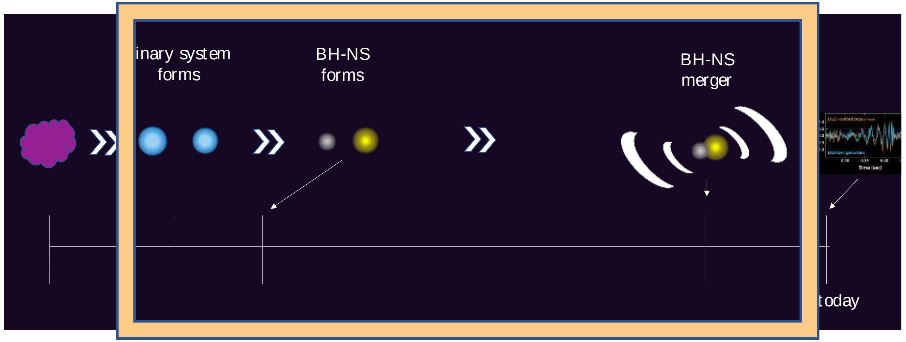

2. (Binary) stellar evolution?

Describes "model for the Universe":

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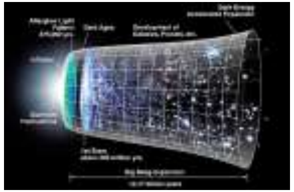
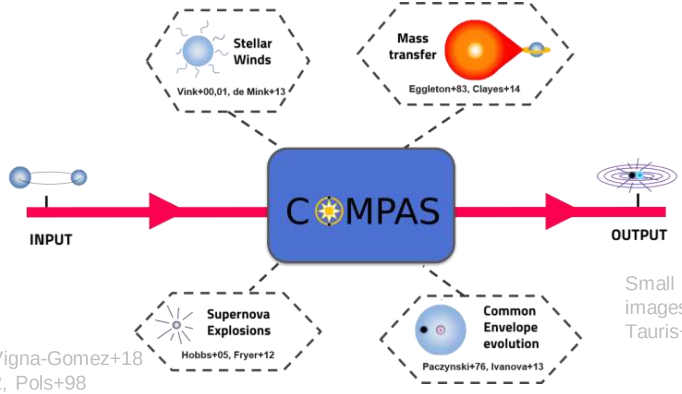
Star formation rate **SFR(z)**

Chemical evolution **Z(z)**



Describes "isolated binary evolution":



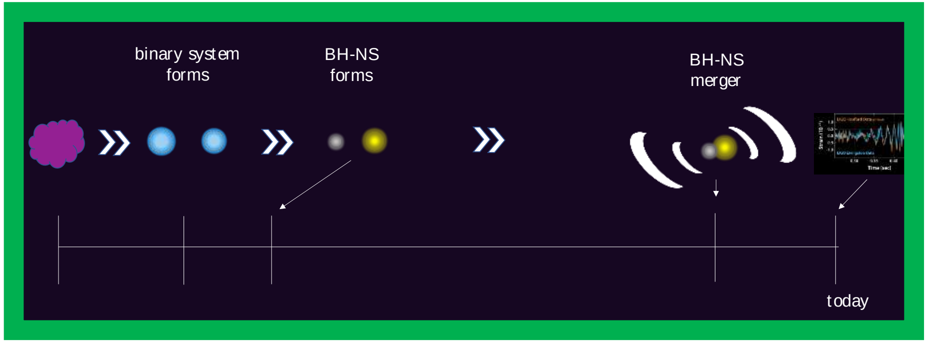
Small images: Tauris+17

cf Chruslinska+19, Belczynski+19 Neijssel+19, Tang+19...

Stevenson+15,17,19, Barrett+18, Vigna-Gomez+18
Based on tracks from Hurley+00,02, Pols+98

We need to understand the combined effect!

1. Star formation history over cosmic time?



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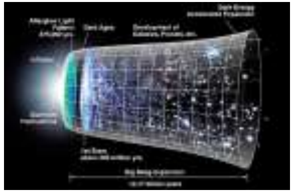

Star formation rate
SFR(z)

Chemical evolution **Z(z)**

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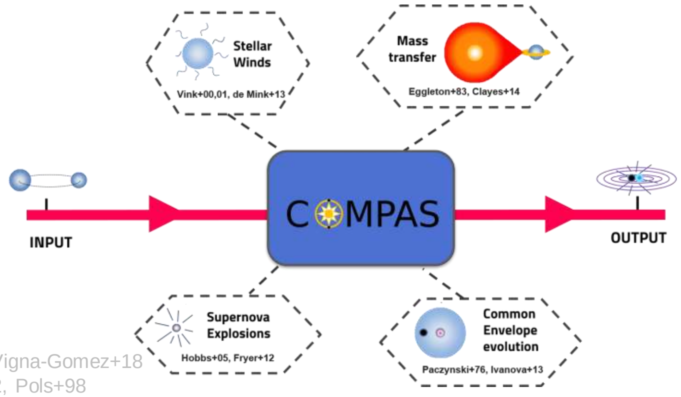

cf Chruslinska+19, Belczynski+19 Neijssel+19, Tang+19...

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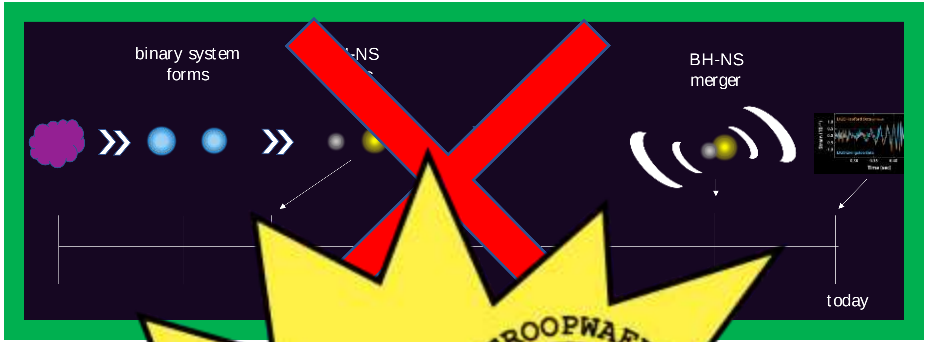


Describes

MSSFR(z...

Star fo...

Requires simulating ma...
metallicities...

New algorithm that speeds up simulations

100x

Broekgaarden+19

And billions of binaries...
= many TBs of data &
>20 000 000 CPU hours...

OUTPUT

Supernova Explosions
Hobbs+05, Fryer+12

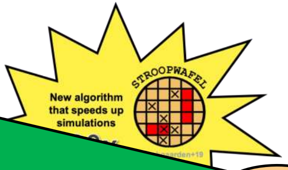
Common Envelope evolution
Paczynski+76, Ivanova+13

cf Chruslinska+19, Belczynski+19 Neijssel+19, Tang+19...

Stevenson+15,17,19, Barrett+18, Vigna-Gomez+18
Based on tracks from Hurley+00,02, Pols+98

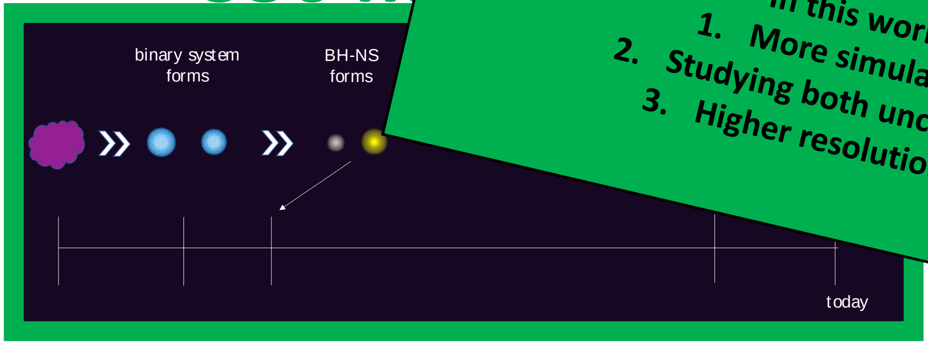
STROOPWAFEL all... to study the impact from b...

336 m...



1. Star formation history over cosmic time?

...) stellar

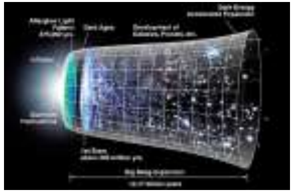


In this work:
1. More simulations
2. Studying both uncertainties
3. Higher resolution data

28 models:

based on Neijssel+19

$$\mathrm{MSSFR}(z_{\mathrm{form}}) = \underbrace{\frac{d^2 M_{\mathrm{SFR}}}{dt_s dV_c}(z_{\mathrm{form}})} \times \underbrace{\frac{dM_{\mathrm{SFR}}}{dZ}(z_{\mathrm{form}})}.$$



Star formation rate
SFR(z)

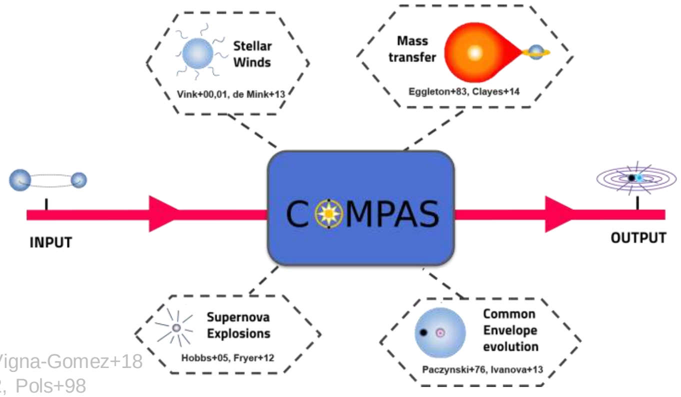
Madau & Dickinson 2014
Strolger +2004
Madau & Fragos 2017

Chemical evolution **Z(z)**

Mass-Z relation:
Langer & Norman 2006 (+offset)
Ma+2016

Galaxy-Stellar-Mass-function:
Panter+2004,
Furlong (single/double Schechter)+2015

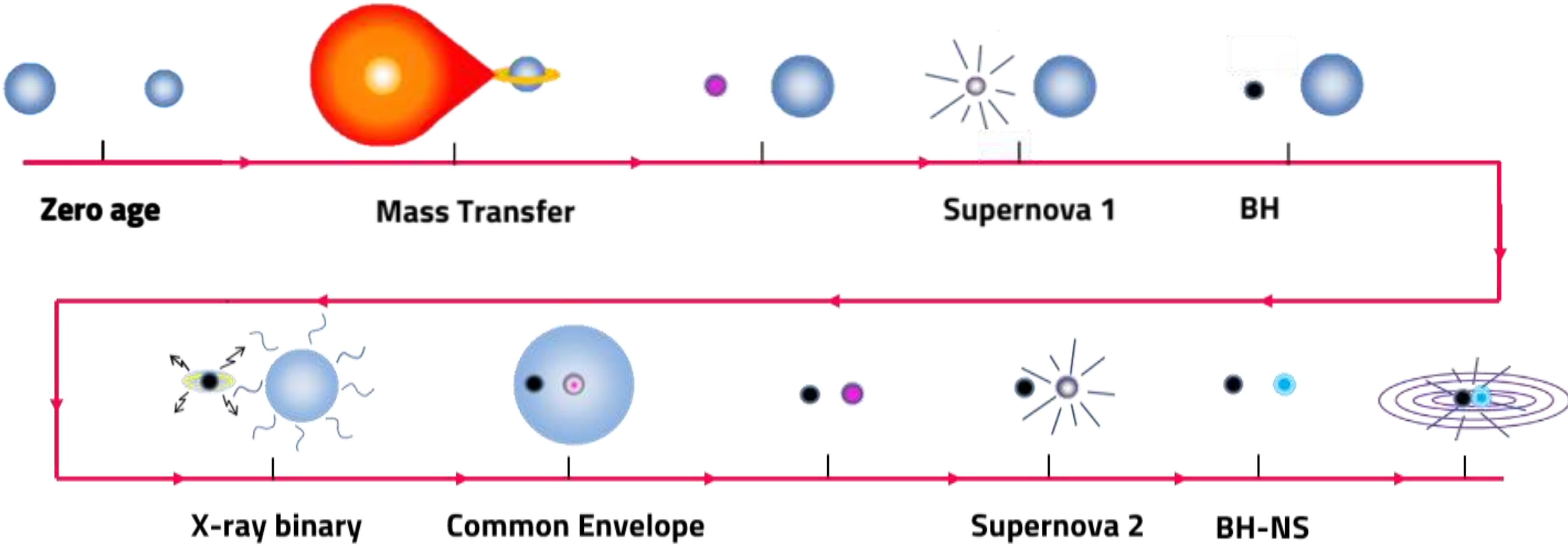
12 models:



Stevenson+15,17,19, Barrett+18, Vigna-Gomez+18
Based on tracks from Hurley+00,02, Pols+98

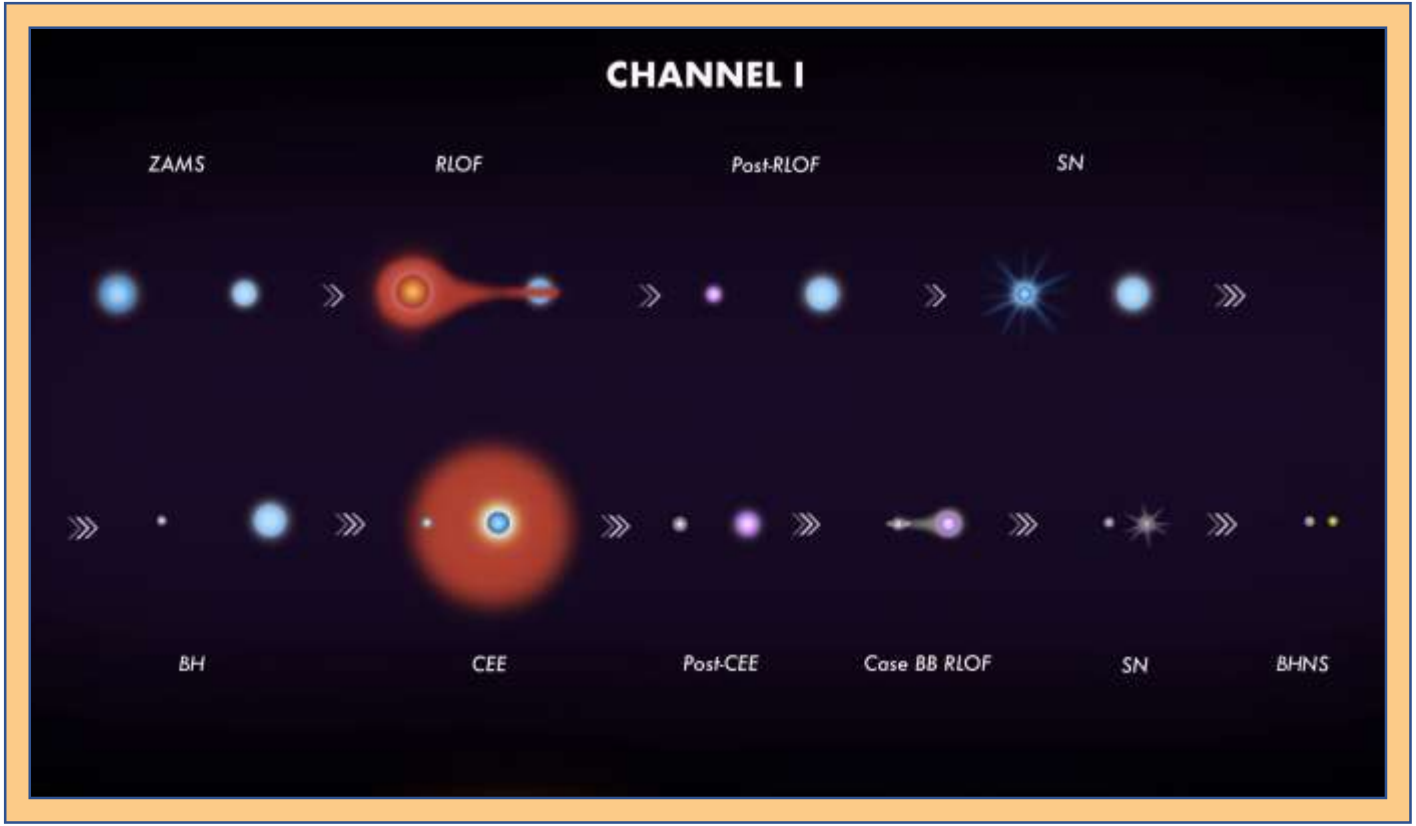
Classic channel BH-NS merger:

e.g. Paczynski+76, Smarr & Blandford+76 | Figure based on Tauris+17



Floor Broekgaarden

Modelling gravitational-wave sources



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How do they form?

$z = 0$

Image not to scale!

e.g. Paczynski+76, Smarr & Blandford+76

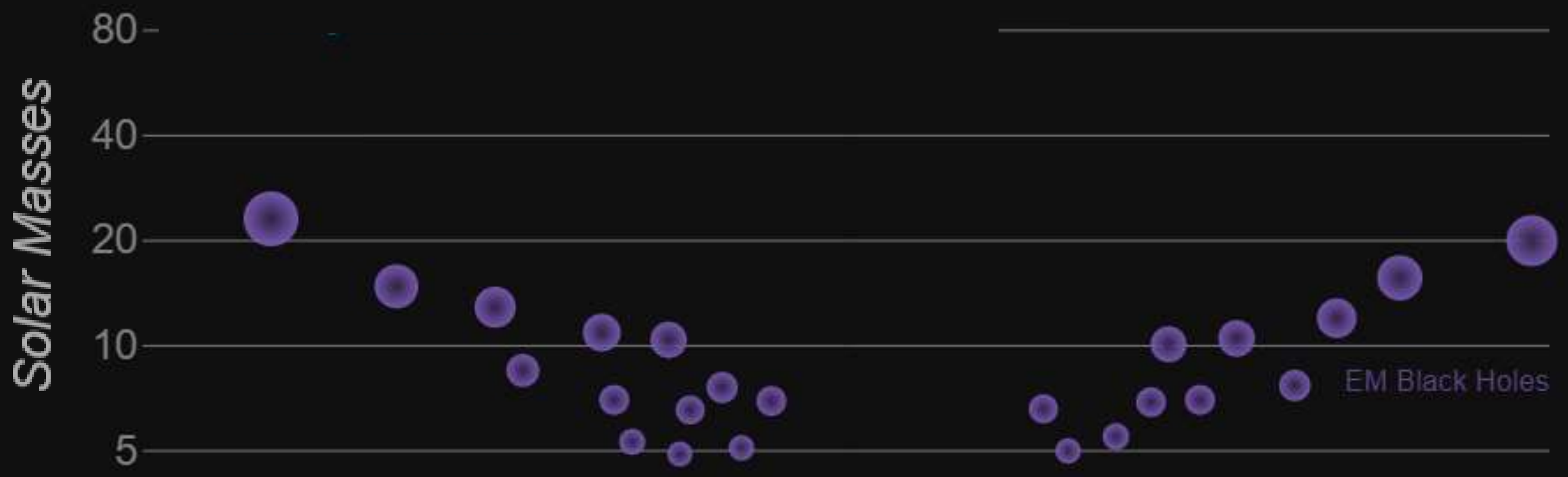
Oher puzzling methods

Q: How many stellar black holes are thought to exist in our Milky Way at this moment?

~100 000 000

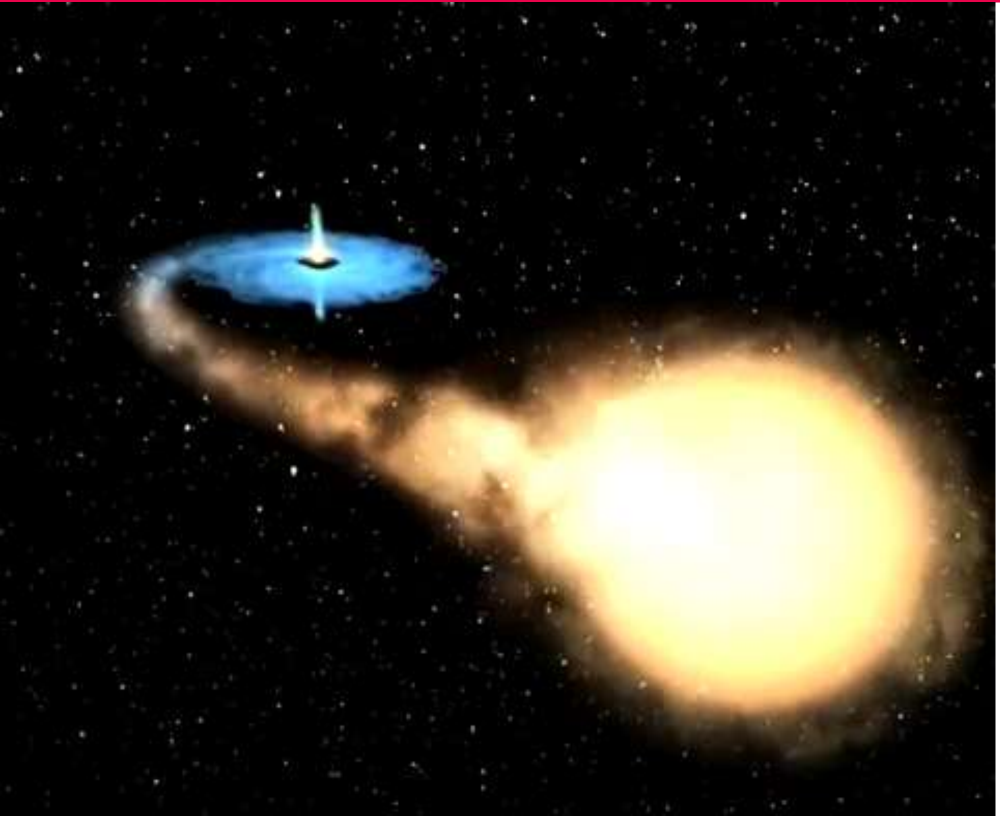
~50 000 000

Up to 2015:
~20 stellar BHs detected with known masses



Q: The first detection of a stellar mass black hole in 1971 (through X-rays)

Bolton +72, Webster and Murdin+72



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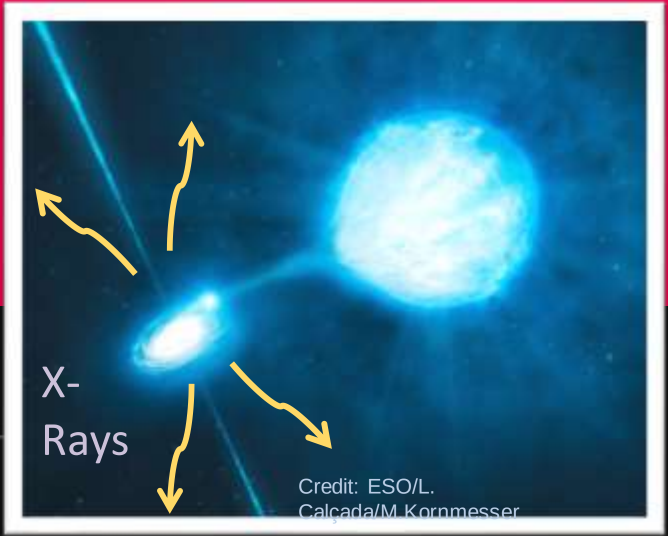
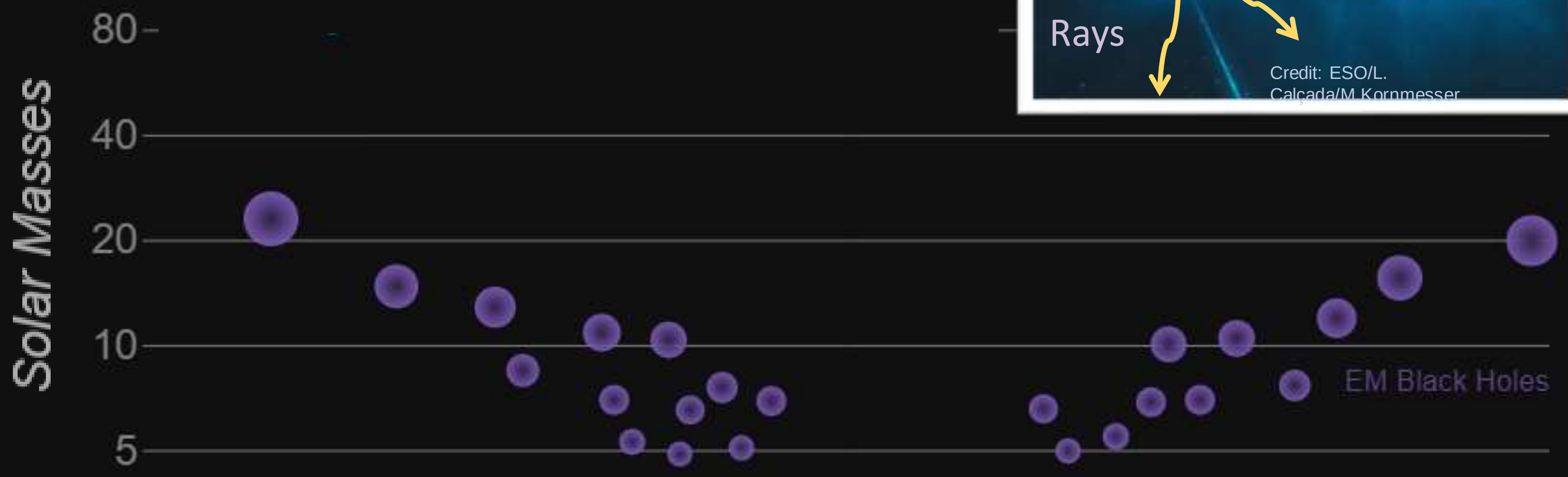
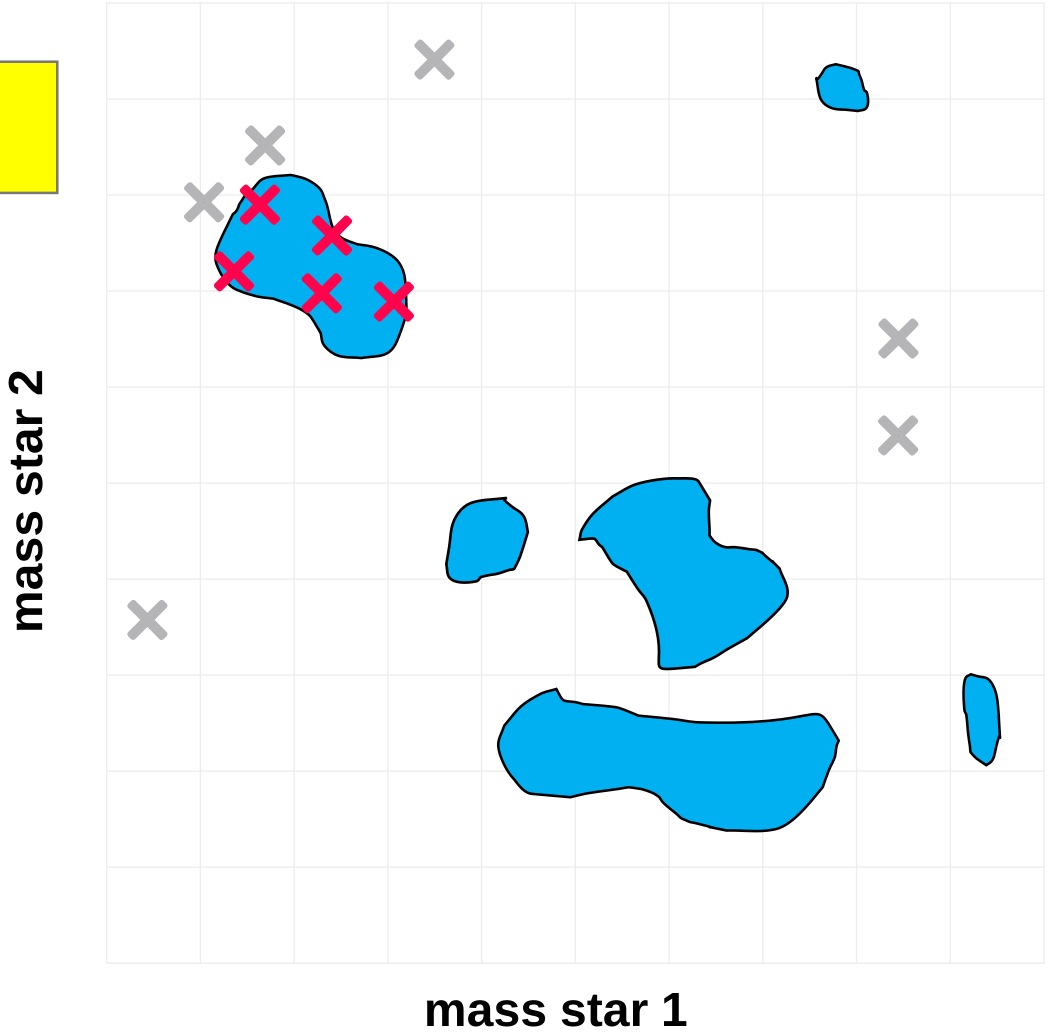
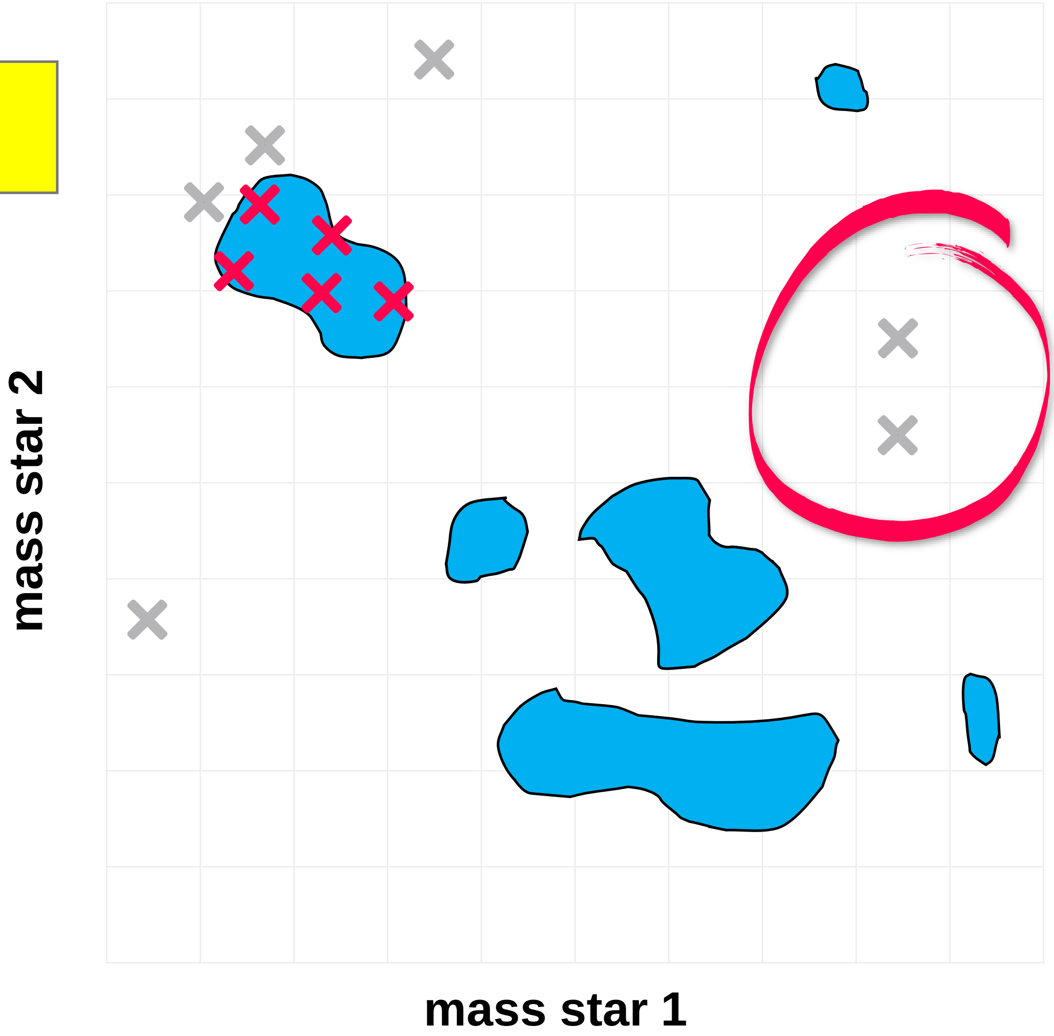




1. “Adaptive learning”

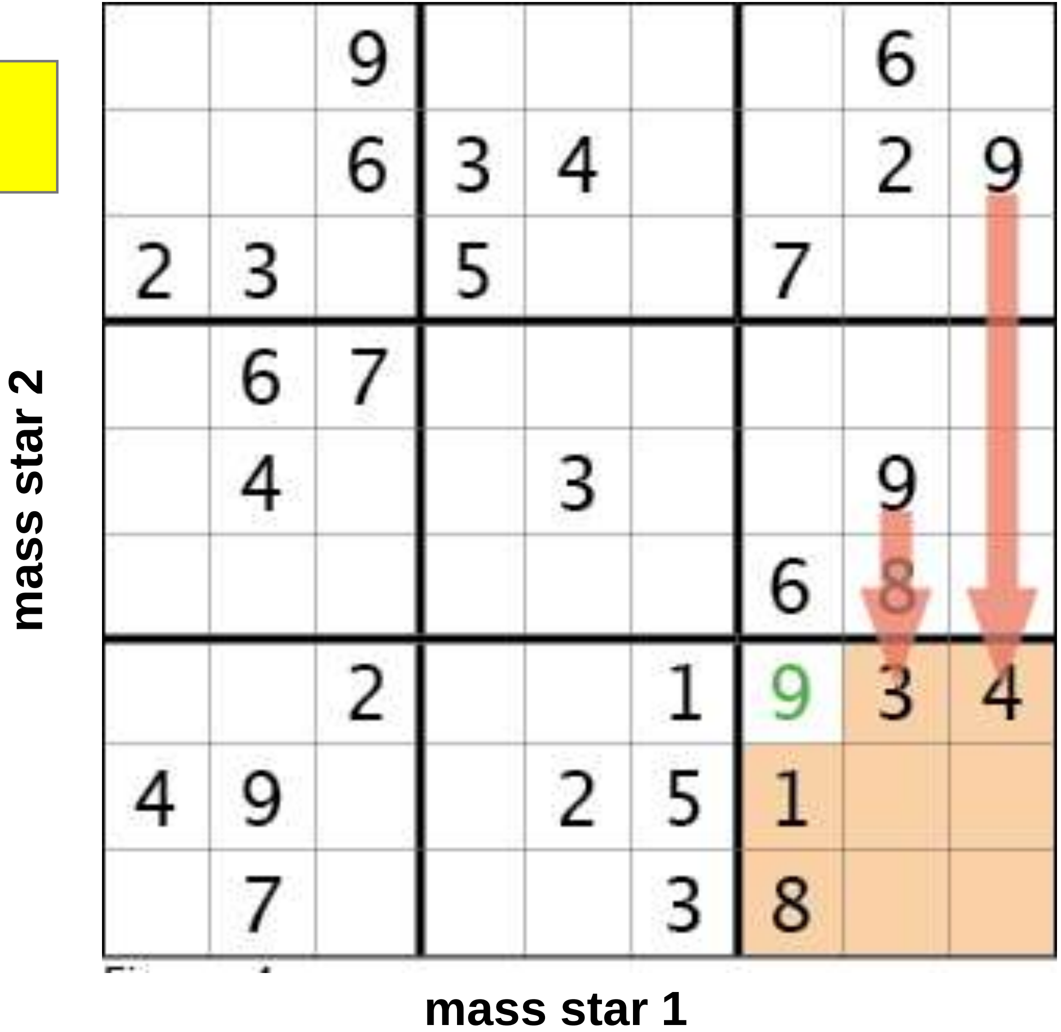


1. "*Adaptive learning*"



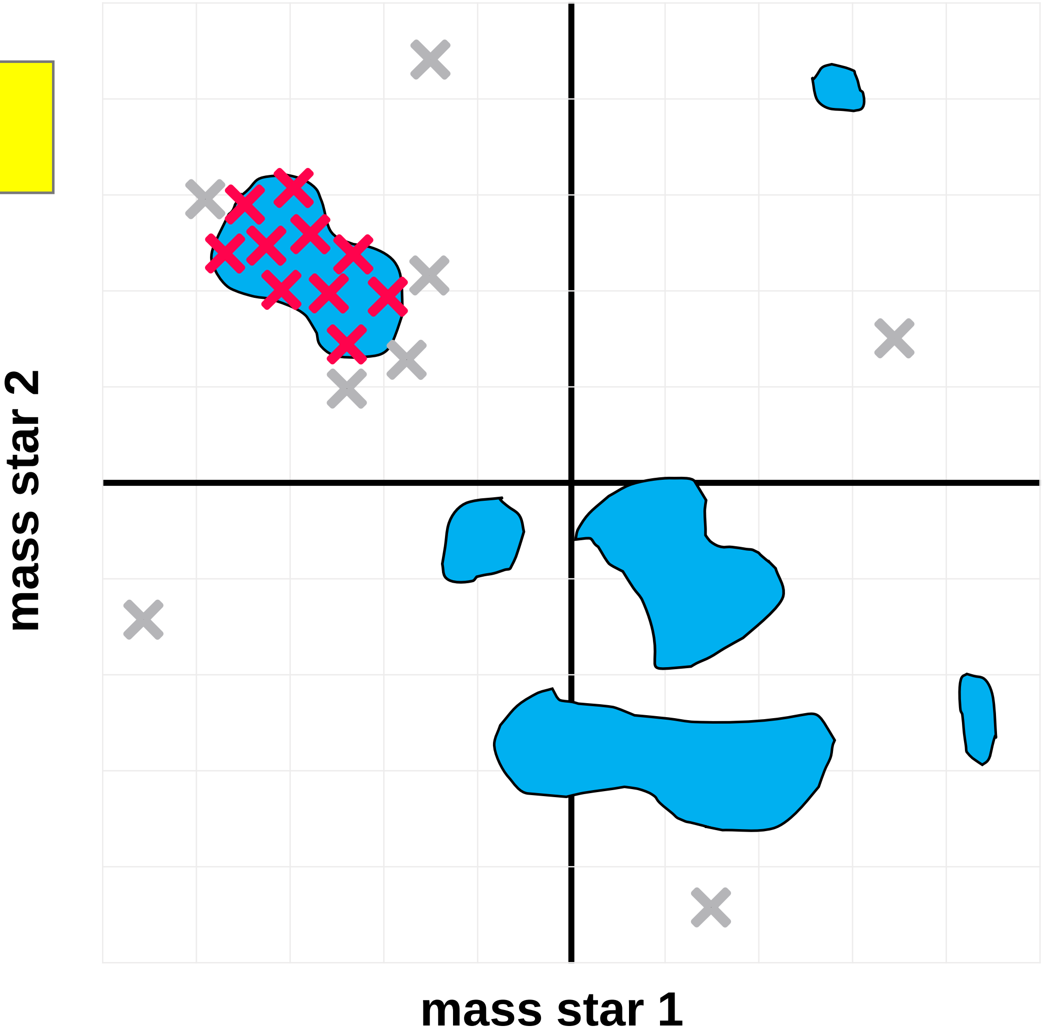
1. “Adaptive learning”

2. Latin hypercube (“Sudoku”) sampling



1. "Adaptive learning"

2. Latin hypercube ("Sudoku") sampling



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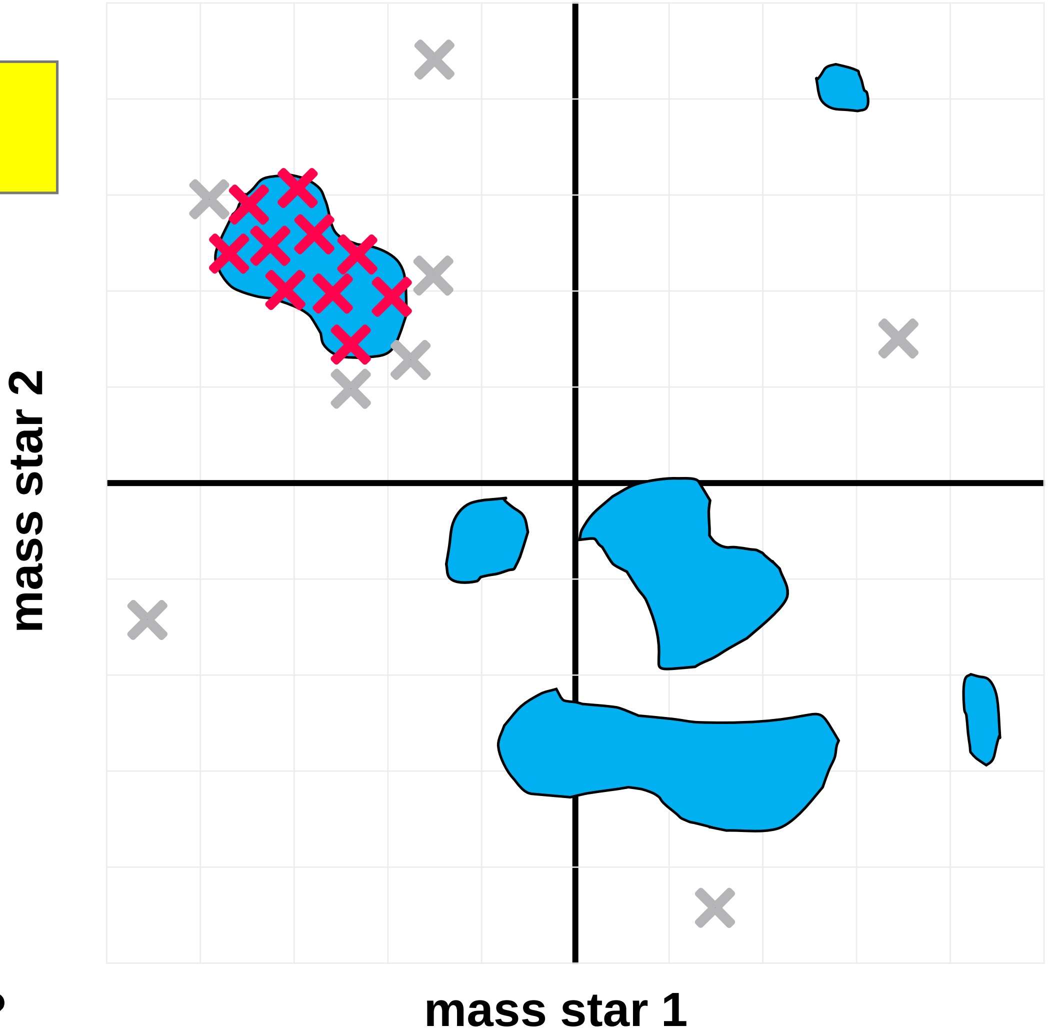
requires

<? >

to complete the game?



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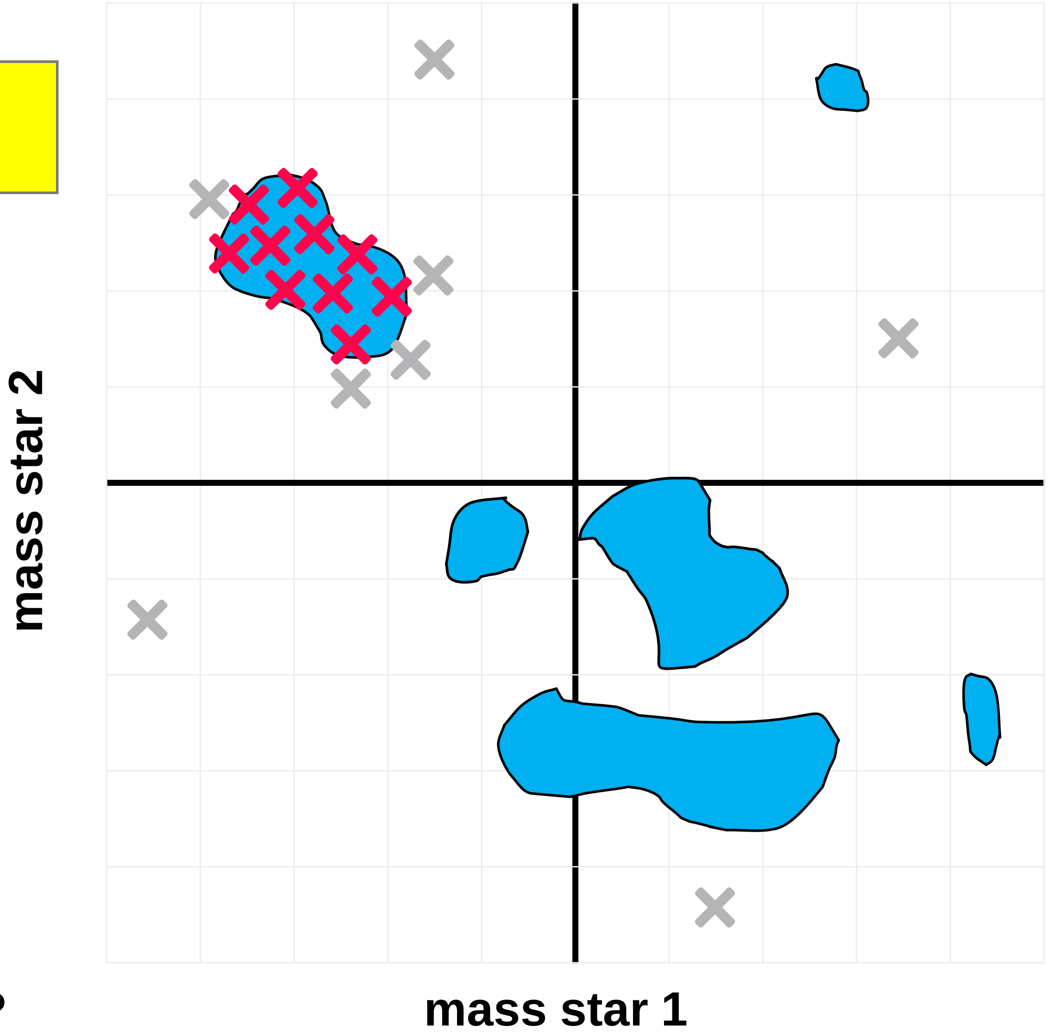

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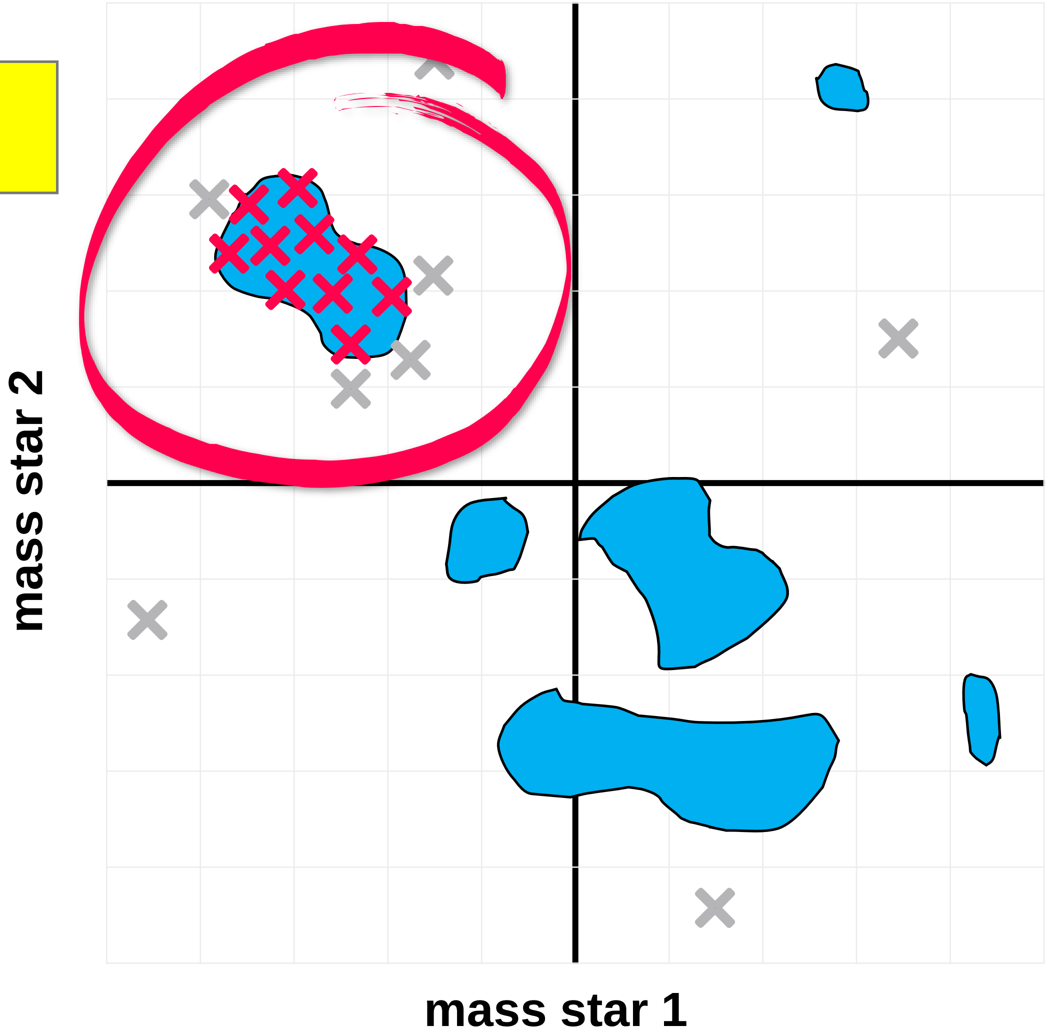

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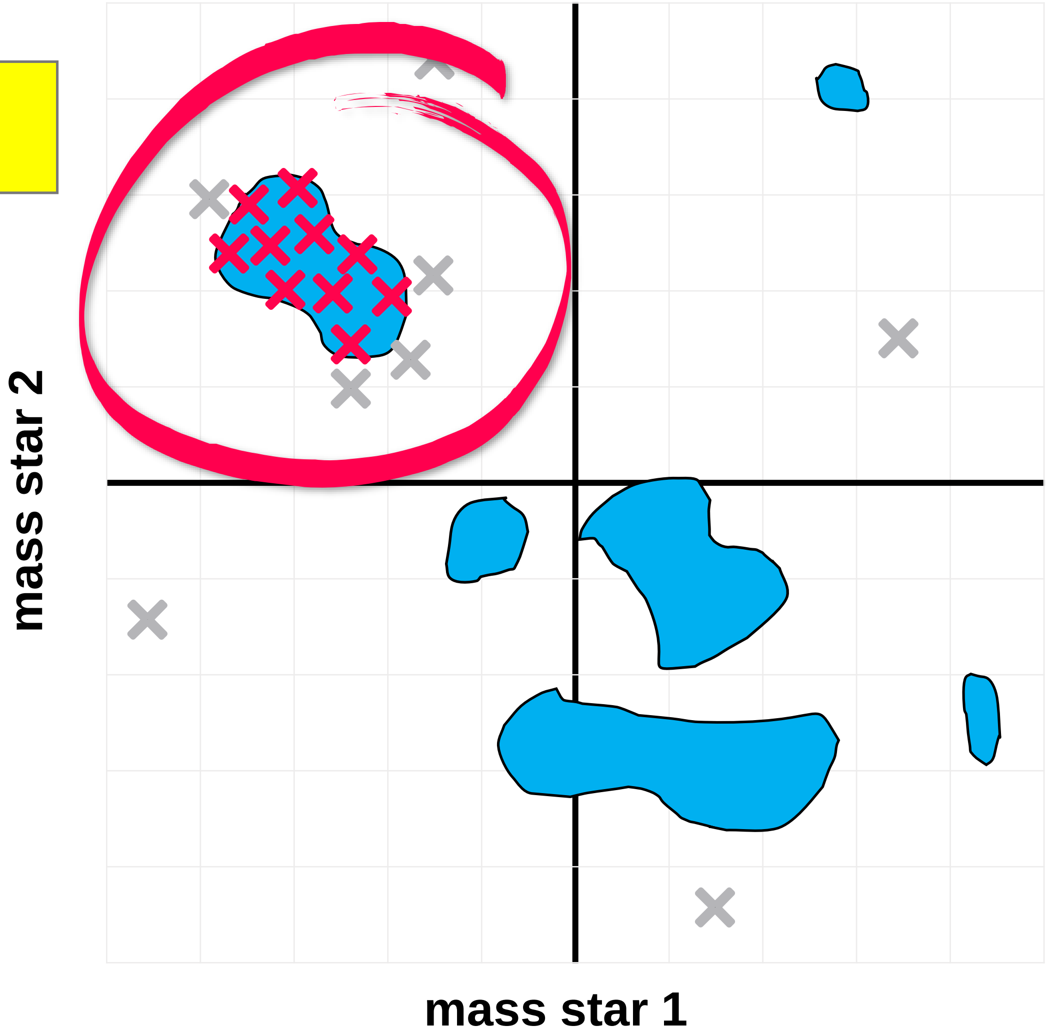
3. *Predict outcome in between ("Emulators")*



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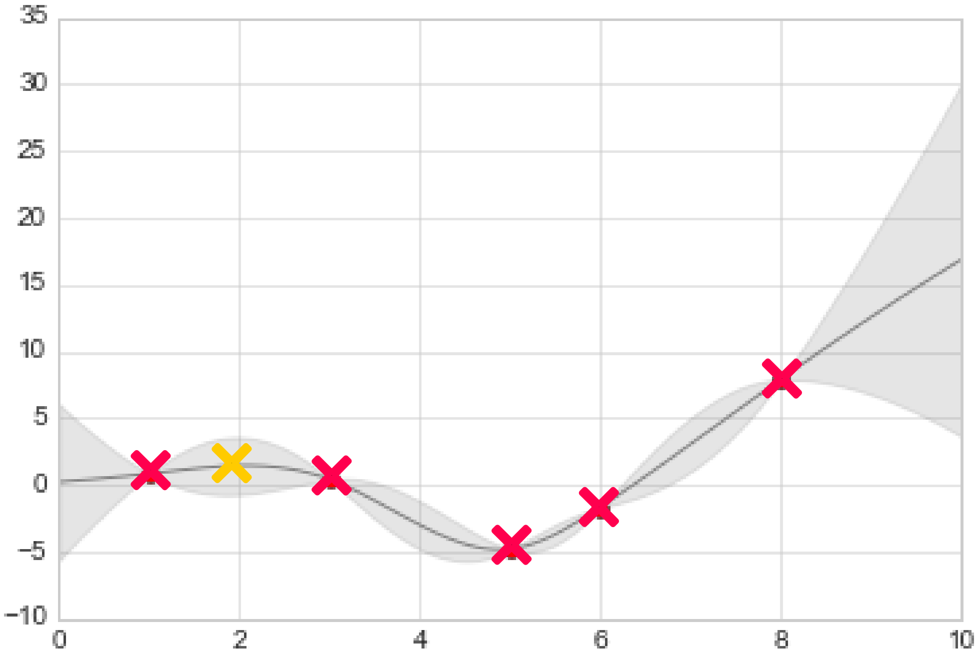
Emulators



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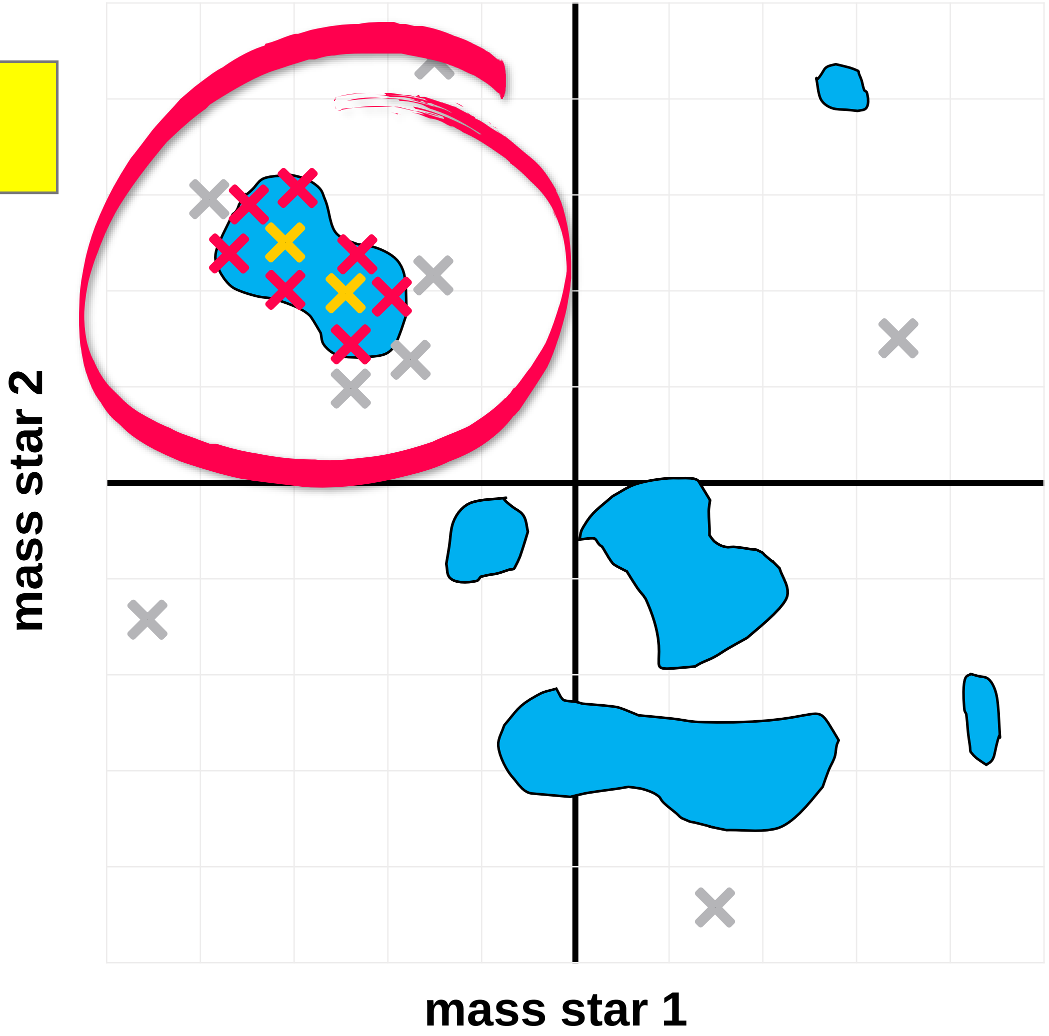
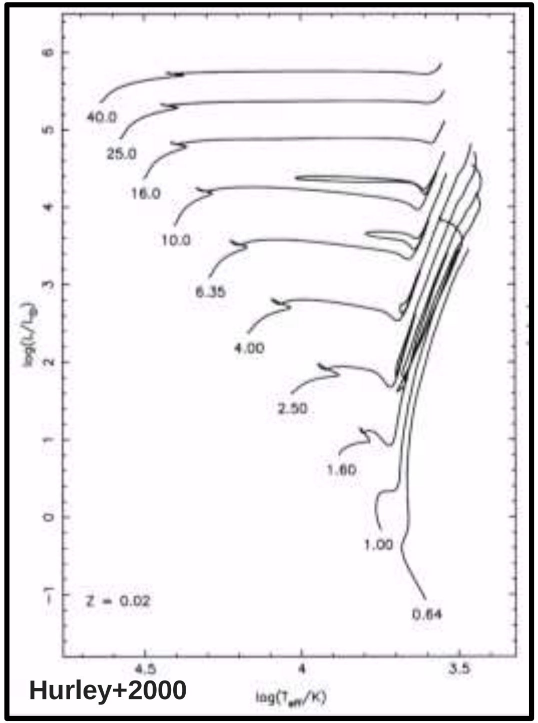


2 ways to implement (single) stellar evolution:

“Full” stellar calculations

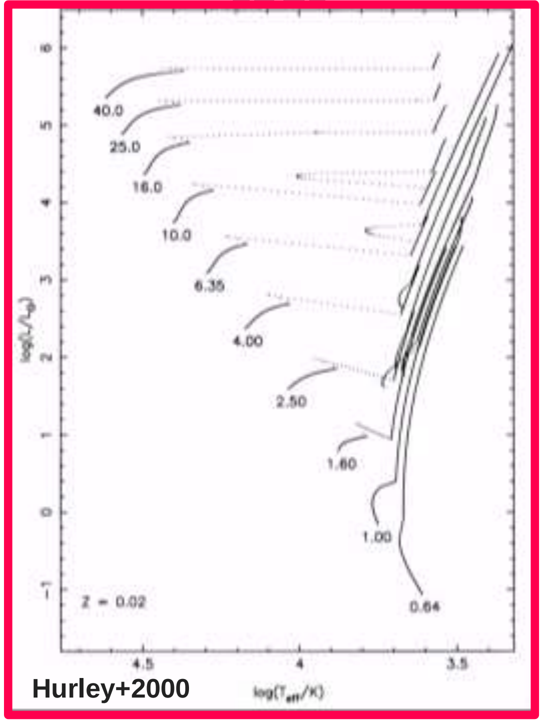
relatively slow



e.g. MESA

Analytical fits or interpolations

fast



e.g. StarTrack, binary_c, COMPAS