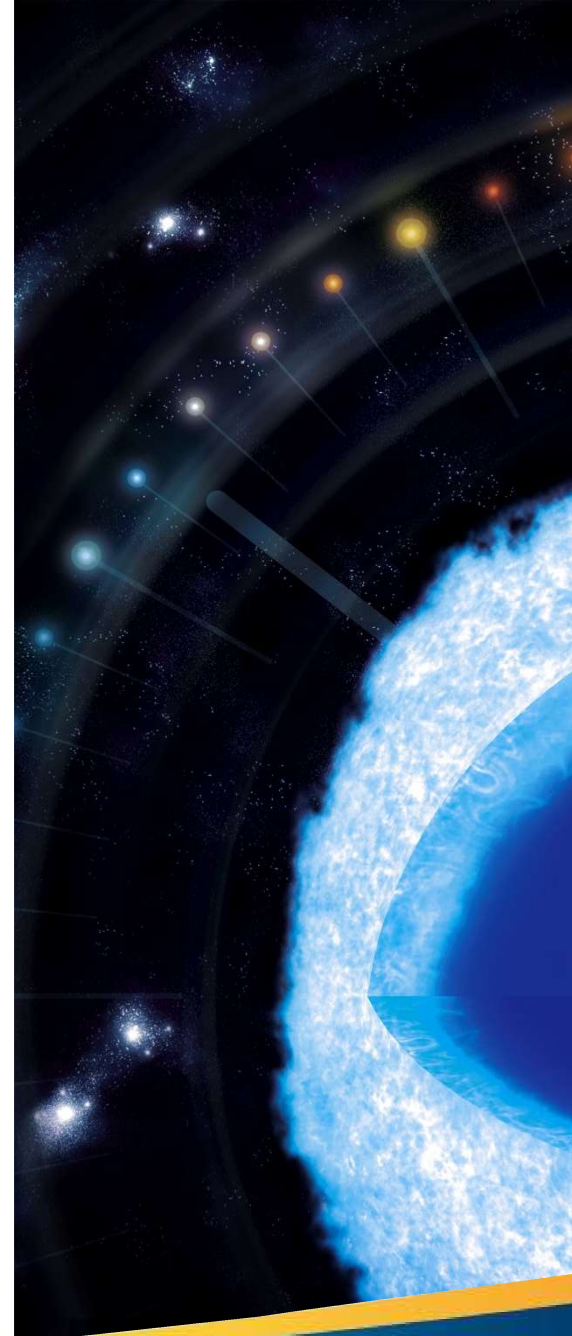
Calculating Melting Curves for Crystallizing Stars

From dense plasma physics to stellar archeology



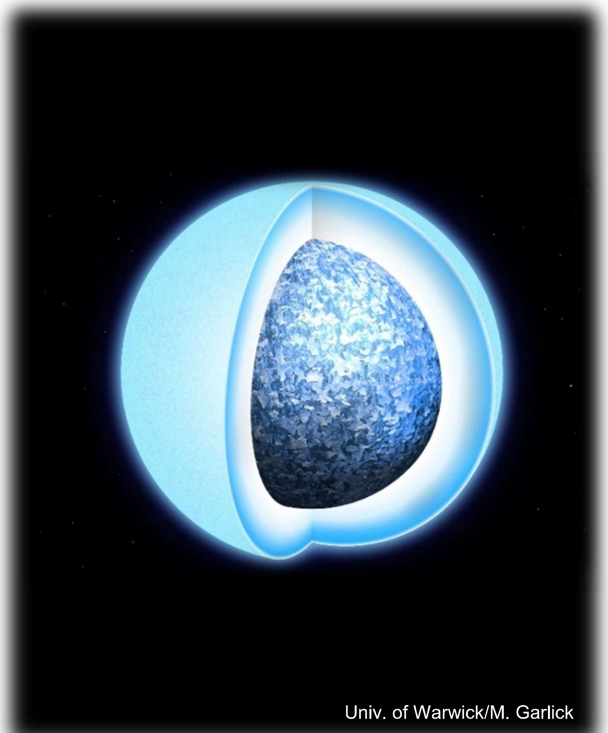
Simon Blouin

LANL

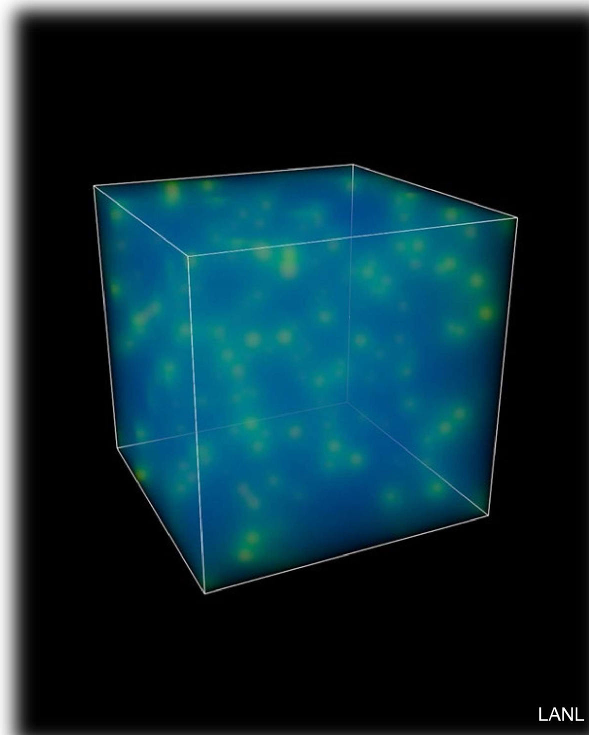
2020-11-05

Slides: LA-UR-20-28803

1. What are white dwarfs and why are they interesting?



2. Core crystallization

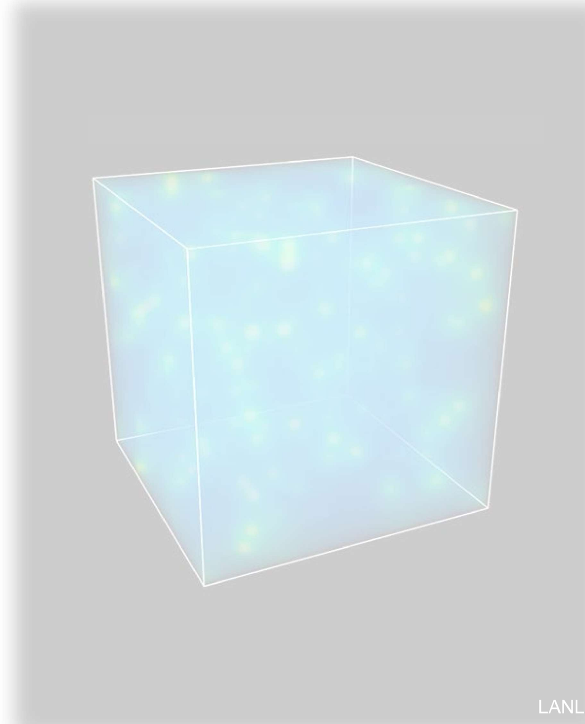


3. Phase diagram calculation

4. C
o

1. What are white dwarfs and why are they interesting?

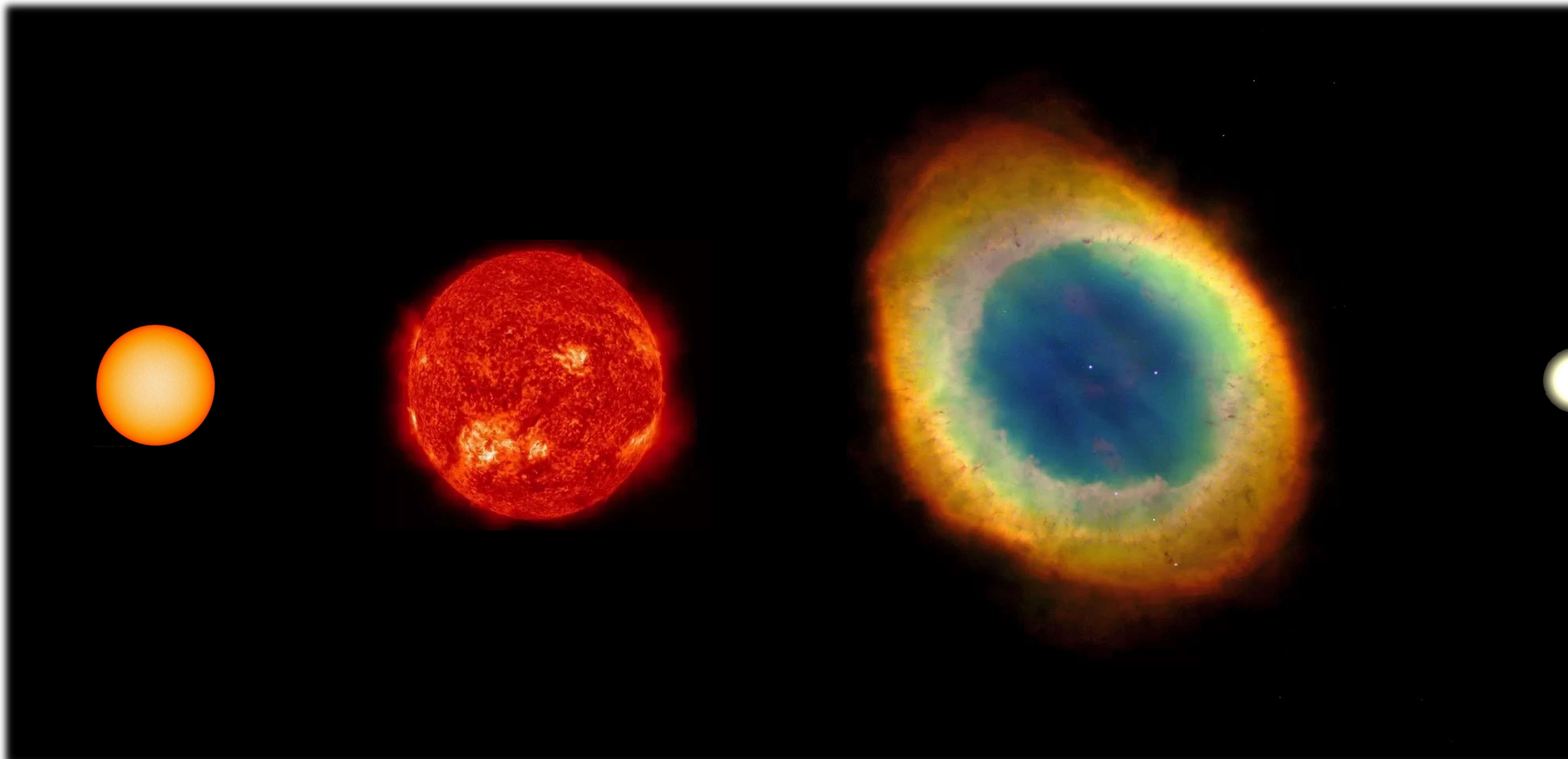
2. Core crystallization



3. Phase diagram calculation

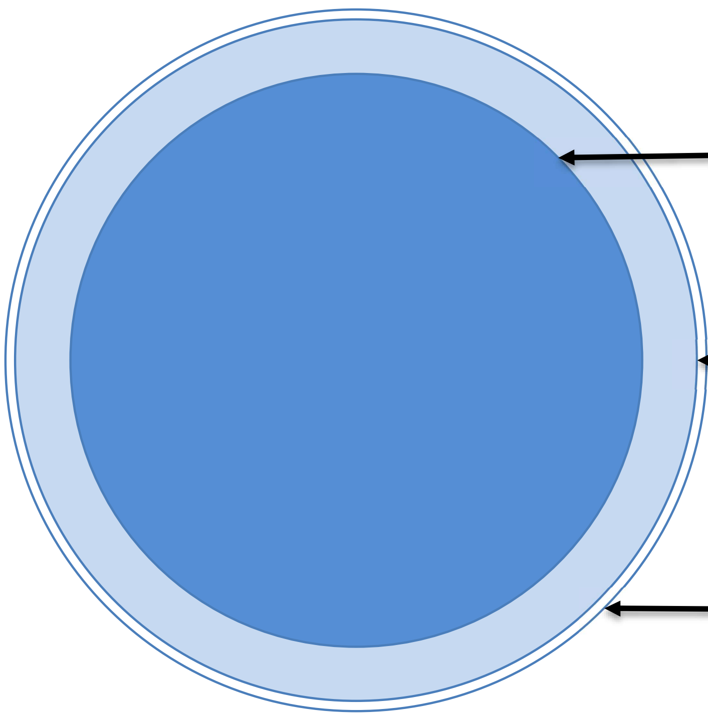
4. C
o

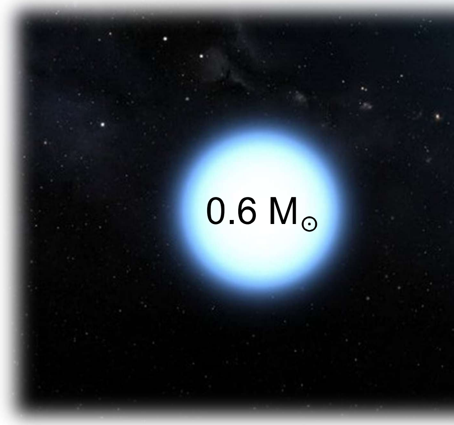
97% of stars end their lives as white dwarfs



NASA/SDO/HMI; N

Anatomy of a white dwarf





C/O core (99% M_{WD})

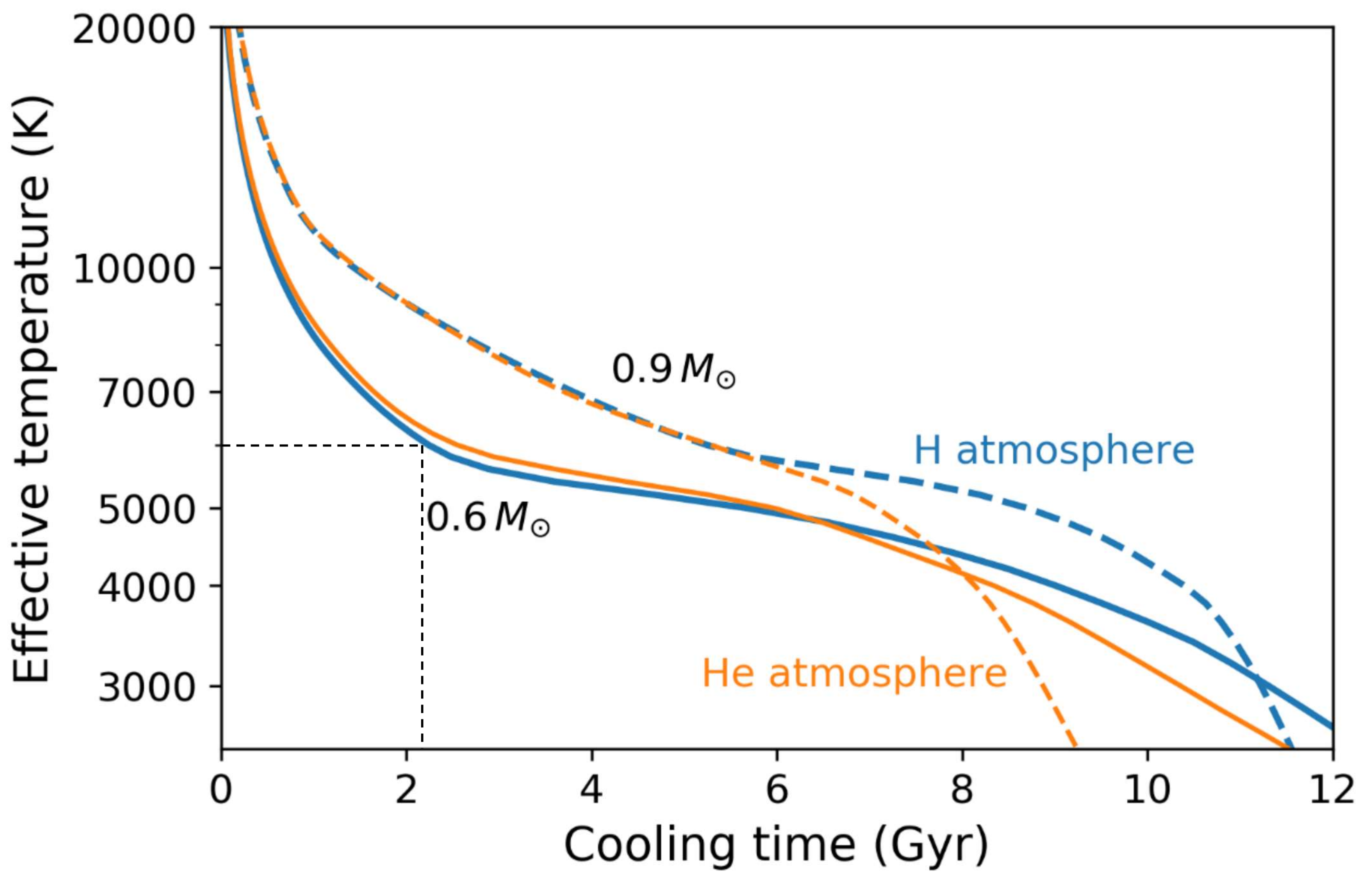
$10^6 – 10^8$ g/cm^3
$10^5 – 10^8$ K

Thick He evelope (10^{-2} M_{WD})

0 – 2 g/cm^3
3000 – 10^5 K

Thin H layer (<10^{-4} M_{WD})

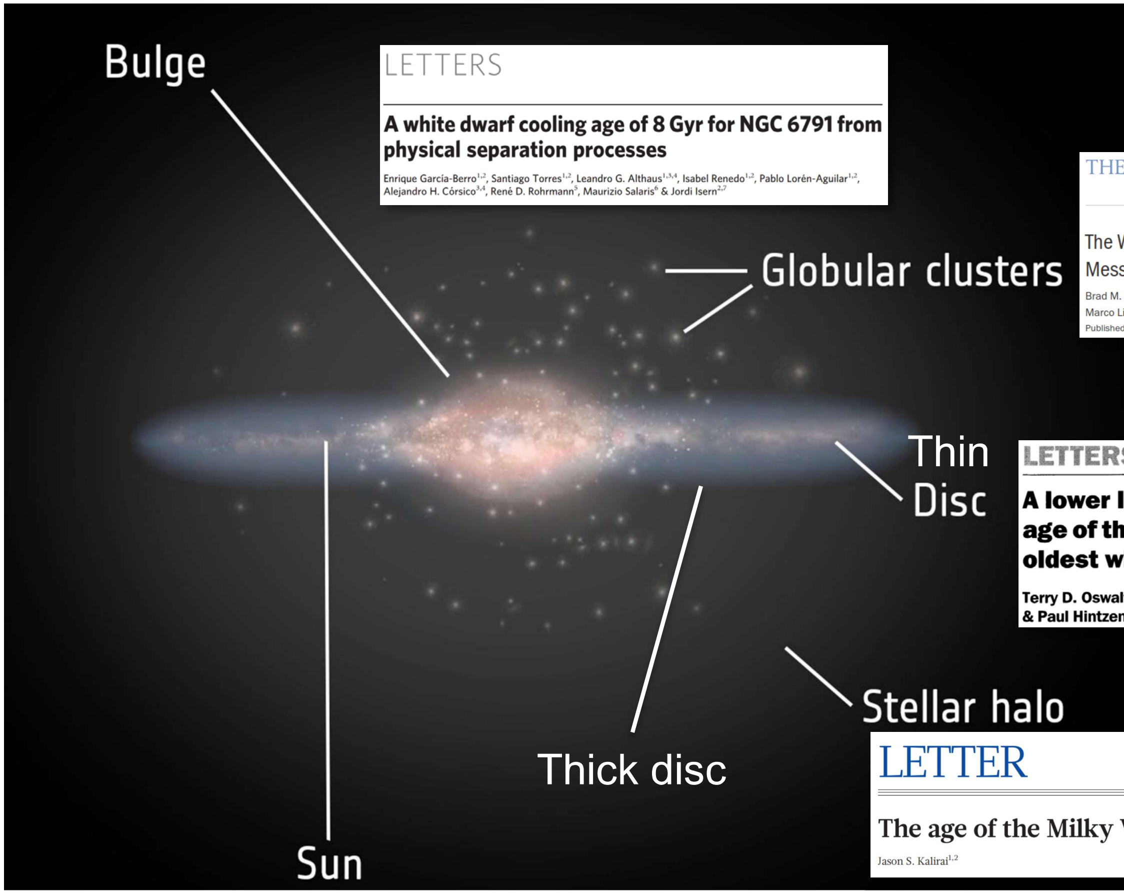
White dwarf cooling



White dwarfs cool dow
monotonically for their
lives

The age of a white dwa
be obtained from its
- temperature
- mass
- atmospheric compos

White dwarf cosmochronology



LETTERS

A white dwarf cooling age of 8 Gyr for NGC 6791 from physical separation processes

Enrique García-Berro[1,2], Santiago Torres[1,2], Leandro G. Althaus[1,3,4], Isabel Renedo[1,2], Pablo Lorén-Aguilar[1,2], Alejandro H. Córsico[3,4], René D. Rohrmann[5], Maurizio Salaris[6] & Jordi Isern[2,7]

THE ASTROPHYSICAL JOURNAL LETTERS

The White Dwarf Cooling Sequence of the Globular Cluster Messier 4*

Brad M. S. Hansen[1,2], James Brewer[3], Greg G. Fahlman[3,4], Brad K. Gibson[5], Rodrigo Ibata[6], Marco Limongi[7], R. Michael Rich[1], Harvey B. Richer[3], Michael M. Shara[8], and Peter B. Stetson[9]

Published 11 July 2002 • © 2002. The American Astronomical Society. All rights reserved. Printed in U.S.A.

LETTERS TO NATURE

A lower limit of 9.5 Gyr on the age of the Galactic disk from the oldest white dwarf stars

Terry D. Oswalt*, J. Allyn Smith*, Matt A. Wood* & Paul Hintzen†

LETTER

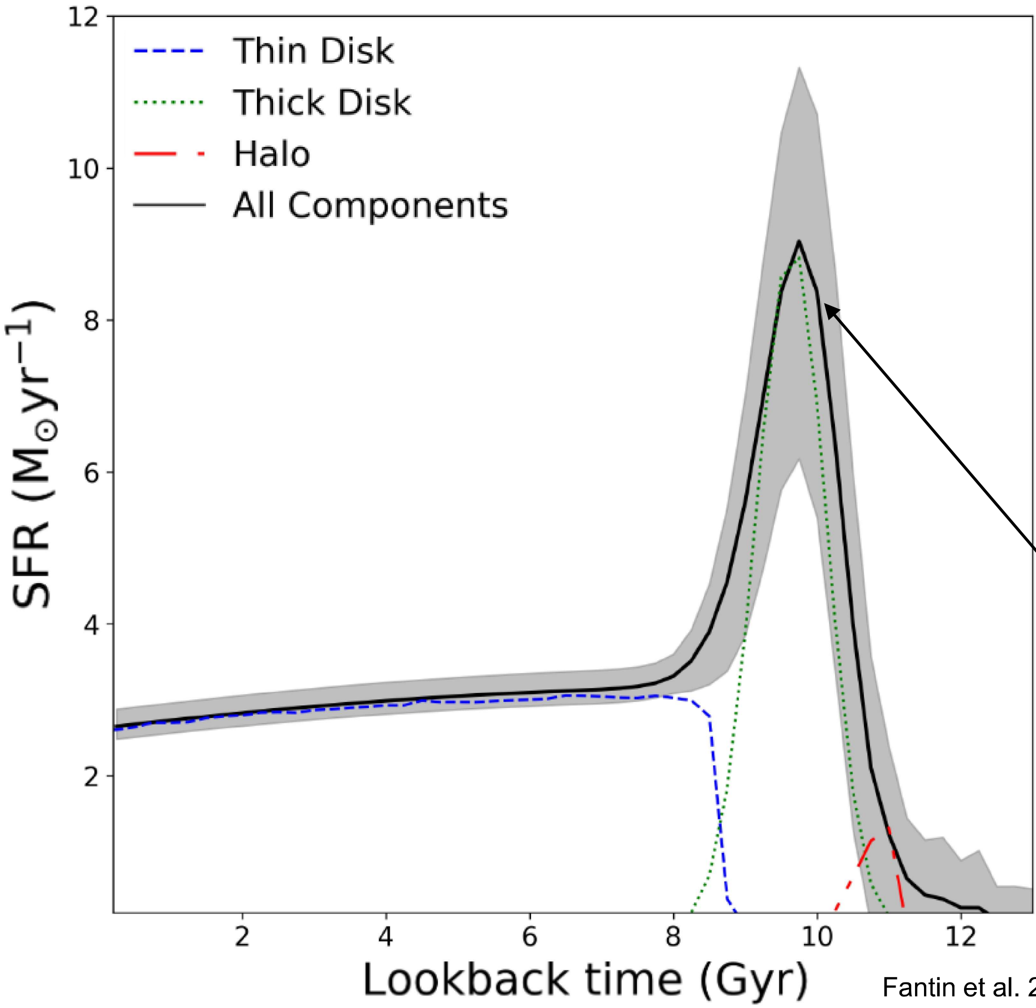
doi:10.1038/nature11062

The age of the Milky Way inner halo

Jason S. Kalirai[1,2]

Using this m
been possibl
measure the
major compo
Galaxy

Stellar archeology



Fantin et al. 2019

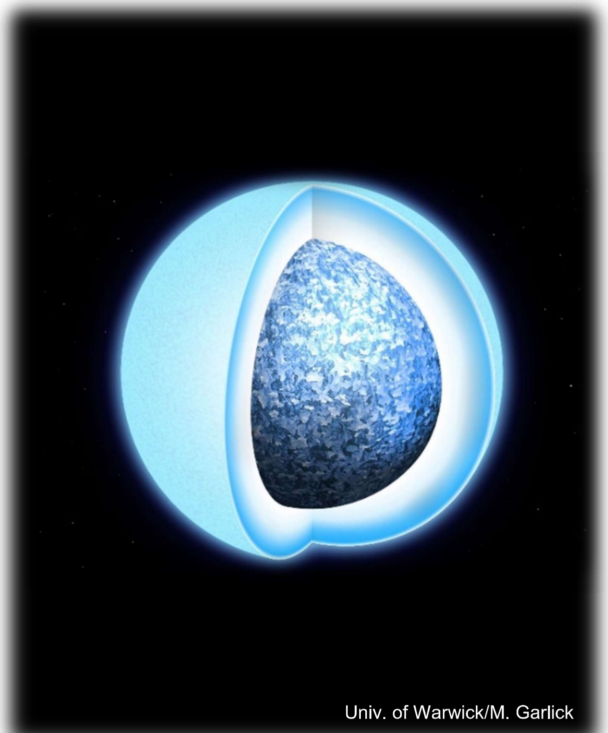
White dwarf cosmochronolog
used to infer stellar formatio
allowing a detailed reconstru
history of our Galaxy

Such applications demand a
cooling models

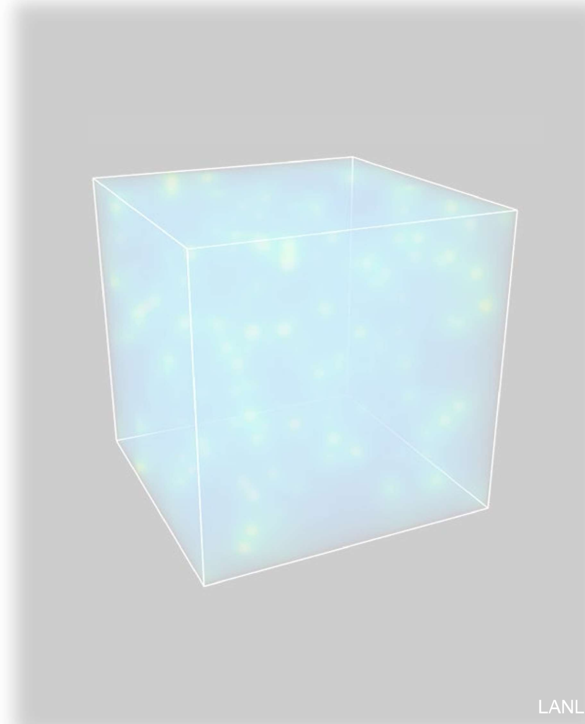
Likely merger with a satellite ga

ESA

1. What are white dwarfs and why are they interesting?


Univ. of Warwick/M. Garlick

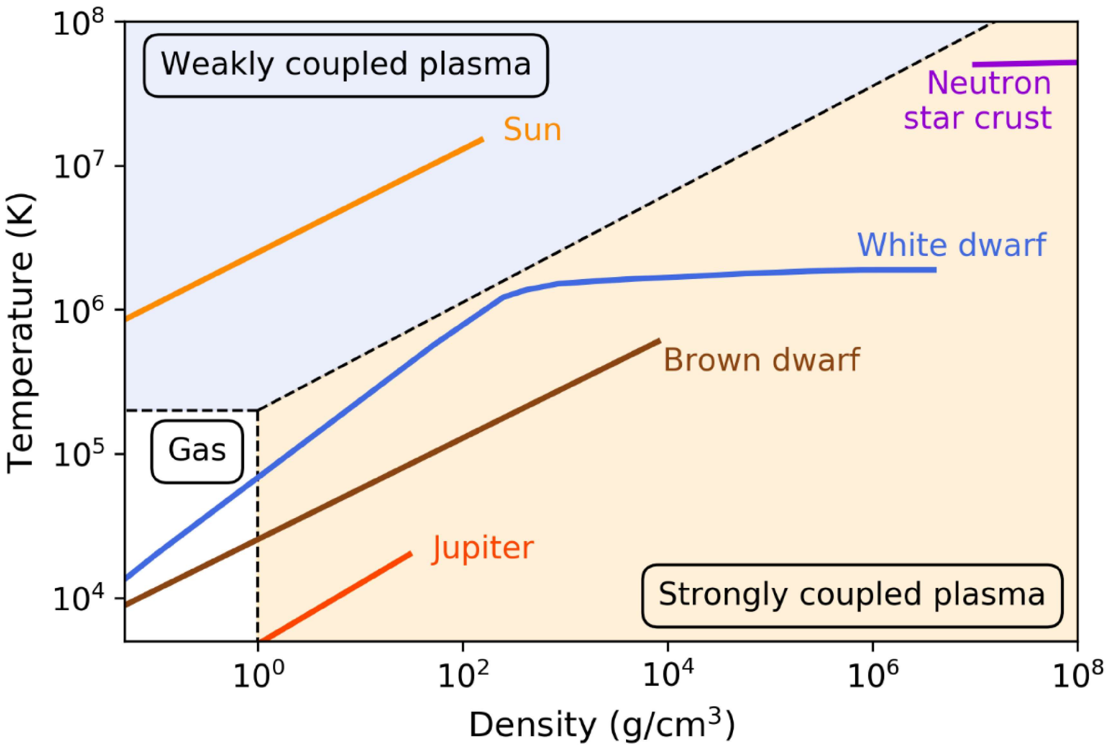
2. Core crystallization

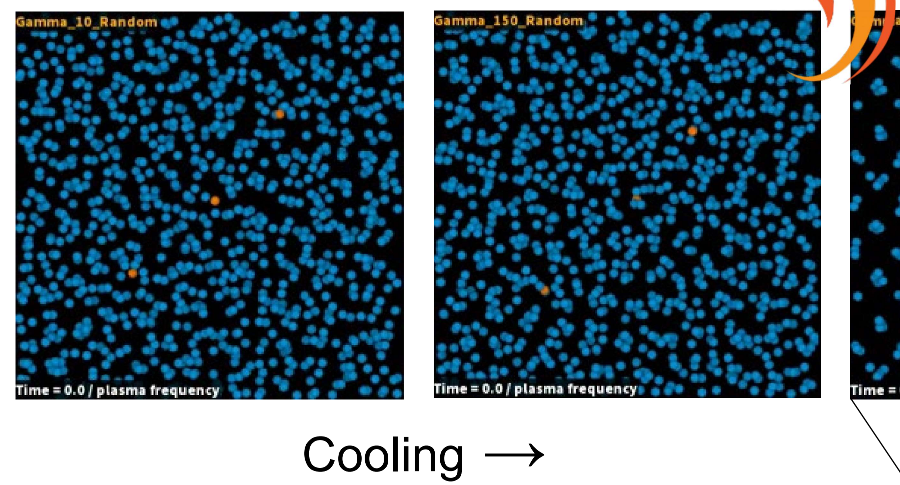

LANL

3. Phase diagram calculation

4. C
o

White dwarf core crystallization



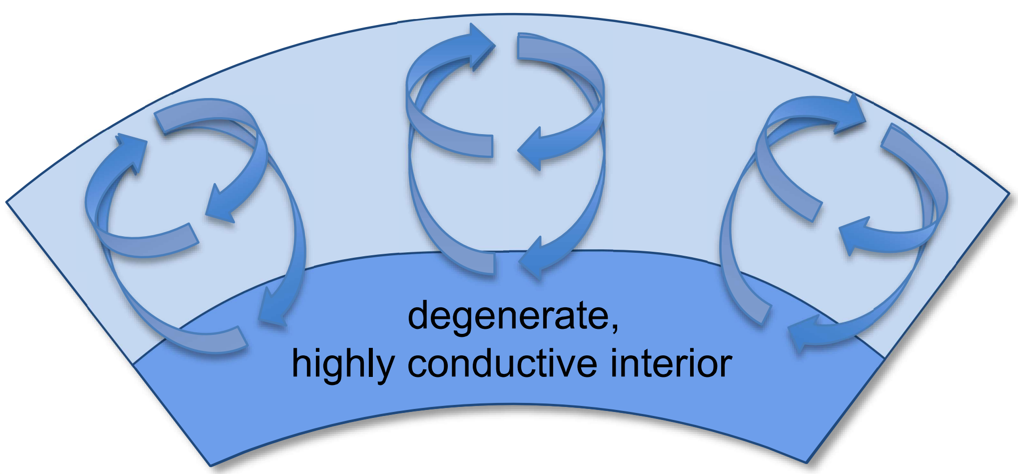


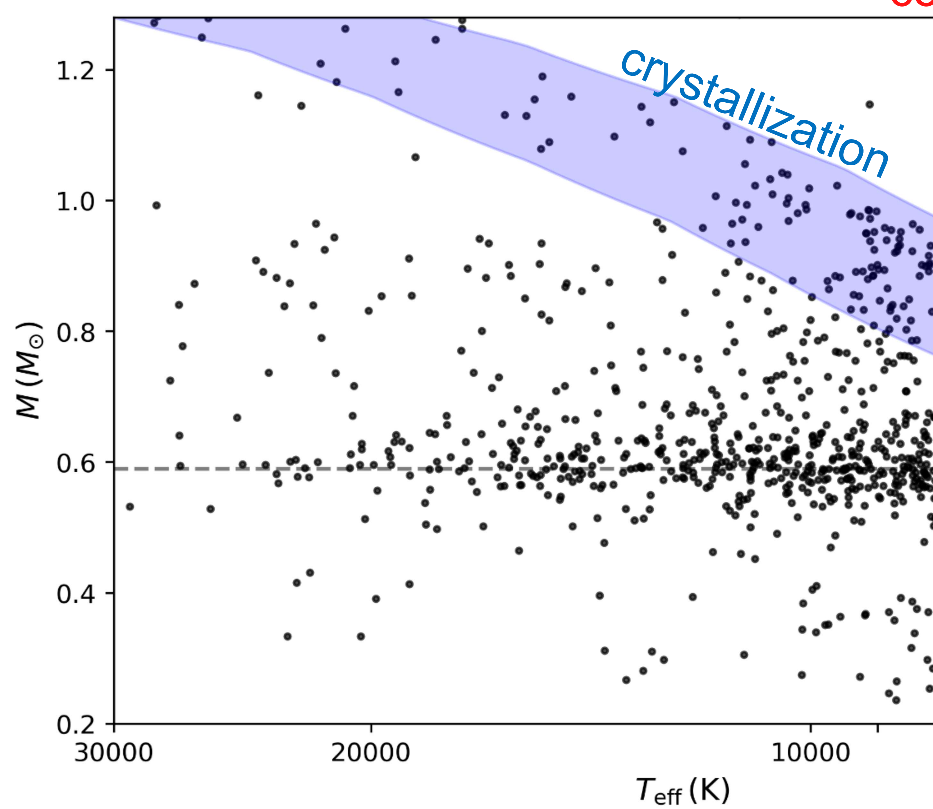
WDs undergo a liquid → solid phase transition that needs to be accurately modeled to unlock the power of precision cosmochronology

Identifying the observational signature of core crystallization

It took 50 years to discover the observational signature of core crystallization

To distinguish the effect of core crystallization from convective coupling, mass measurements were needed



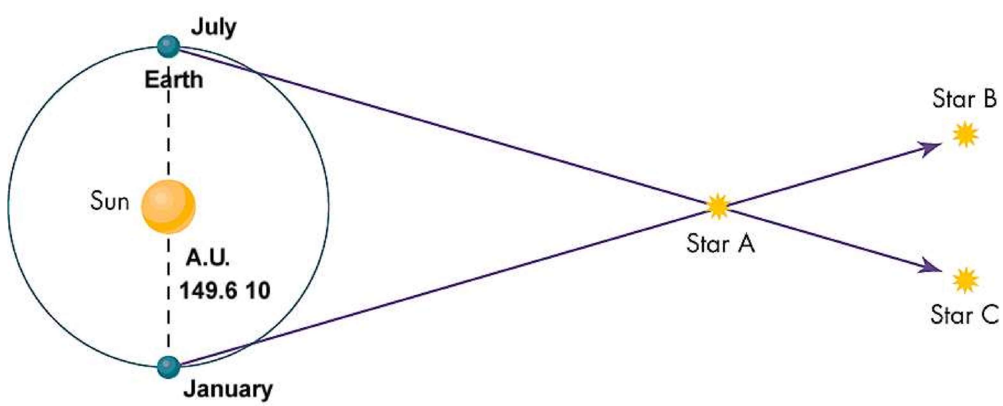


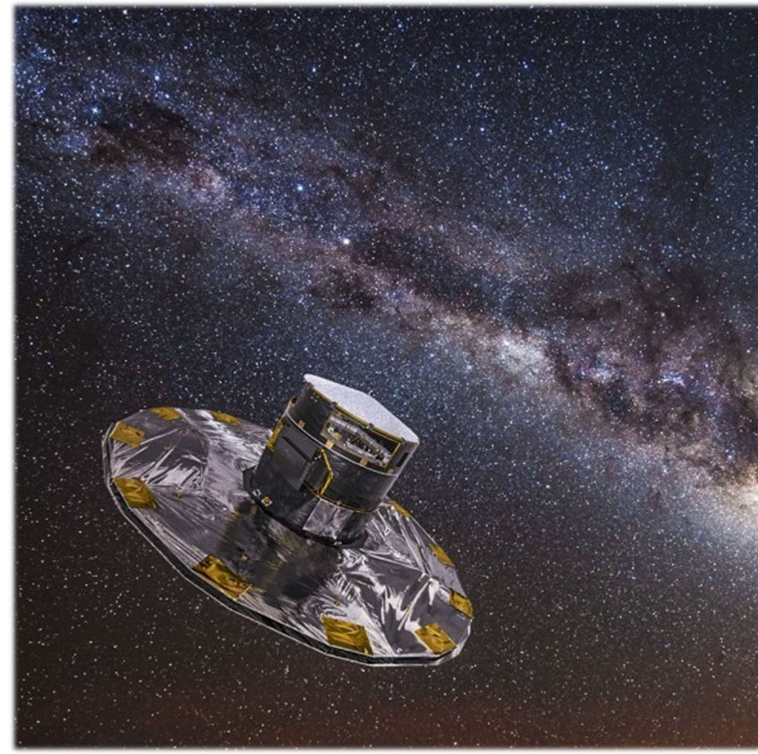
How the Gaia satellite provided mass measurement

ESA's Gaia satellite has increased by a factor of 10 the number of known white dwarfs (now ~250,000)

Launched in 2013, first major data release in 2018

Gaia measures stellar parallaxes with an unprecedented accuracy



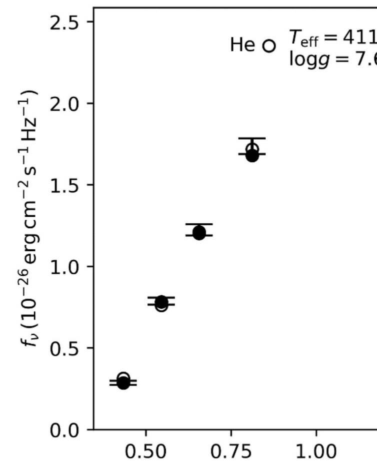


How the Gaia satellite provided mass measurement

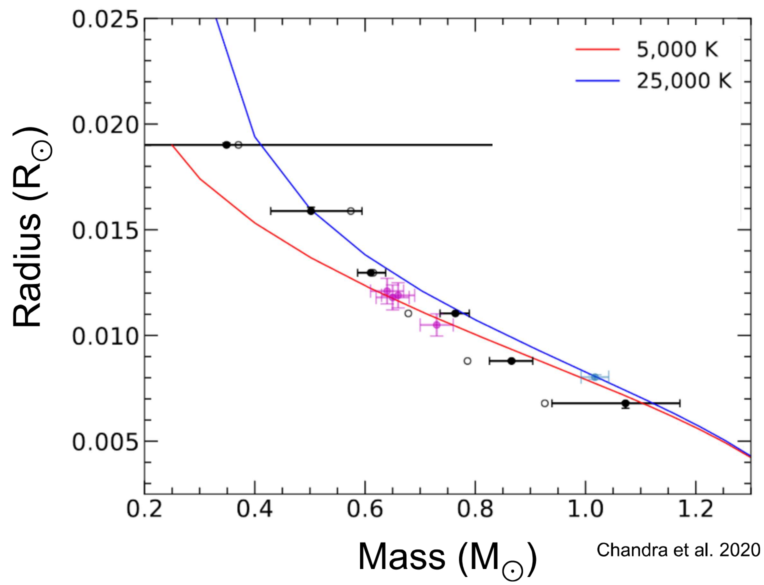
$$\text{Observed flux} = \frac{\pi R^2}{D^2} \times \text{Surface flux}$$

Gaia measurements

Model at



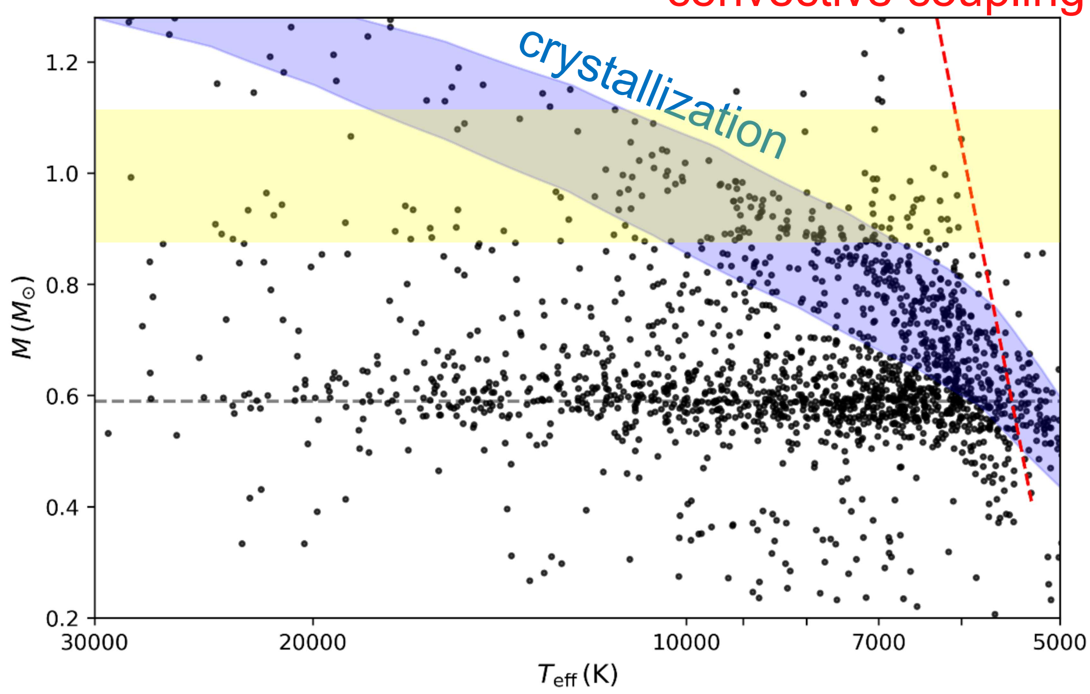
WDs follow a well-defined mass-radius relationship

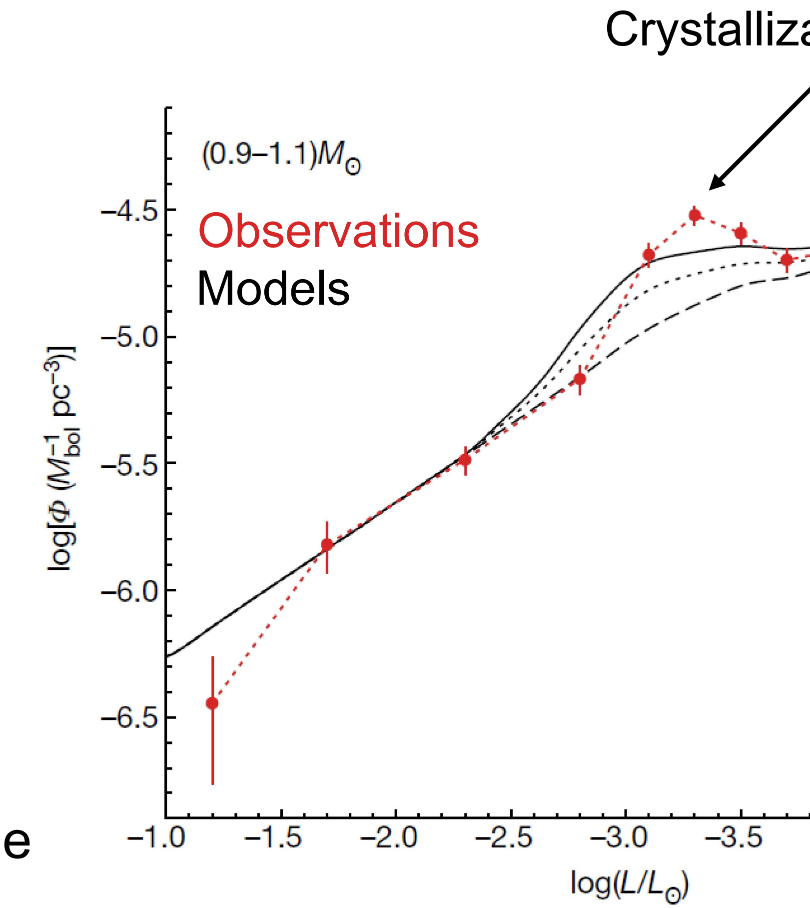


Chandra et al. 2020

In the pre-Gaia era, there was a degeneracy between R and D for most white dwarfs

The signature of core crystallization

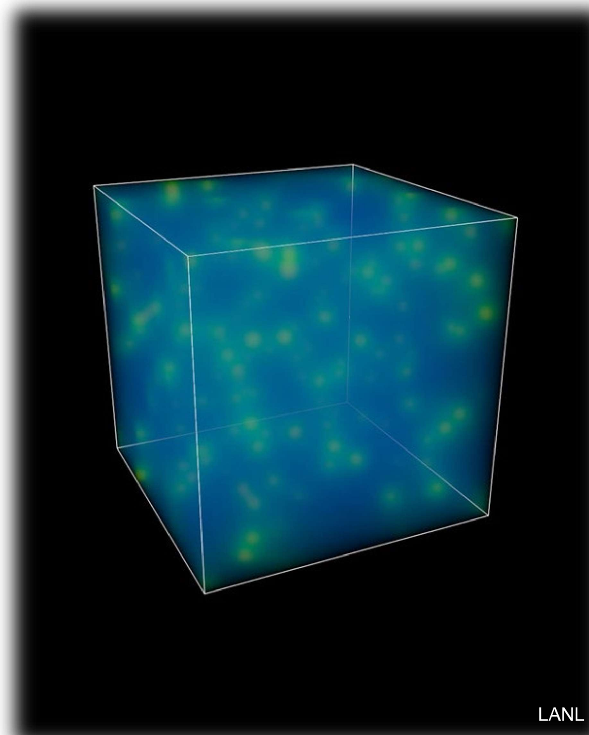




The effect of core crystallization is best seen in the luminosity function of massive WDs

1. What are white dwarfs and why are they interesting?

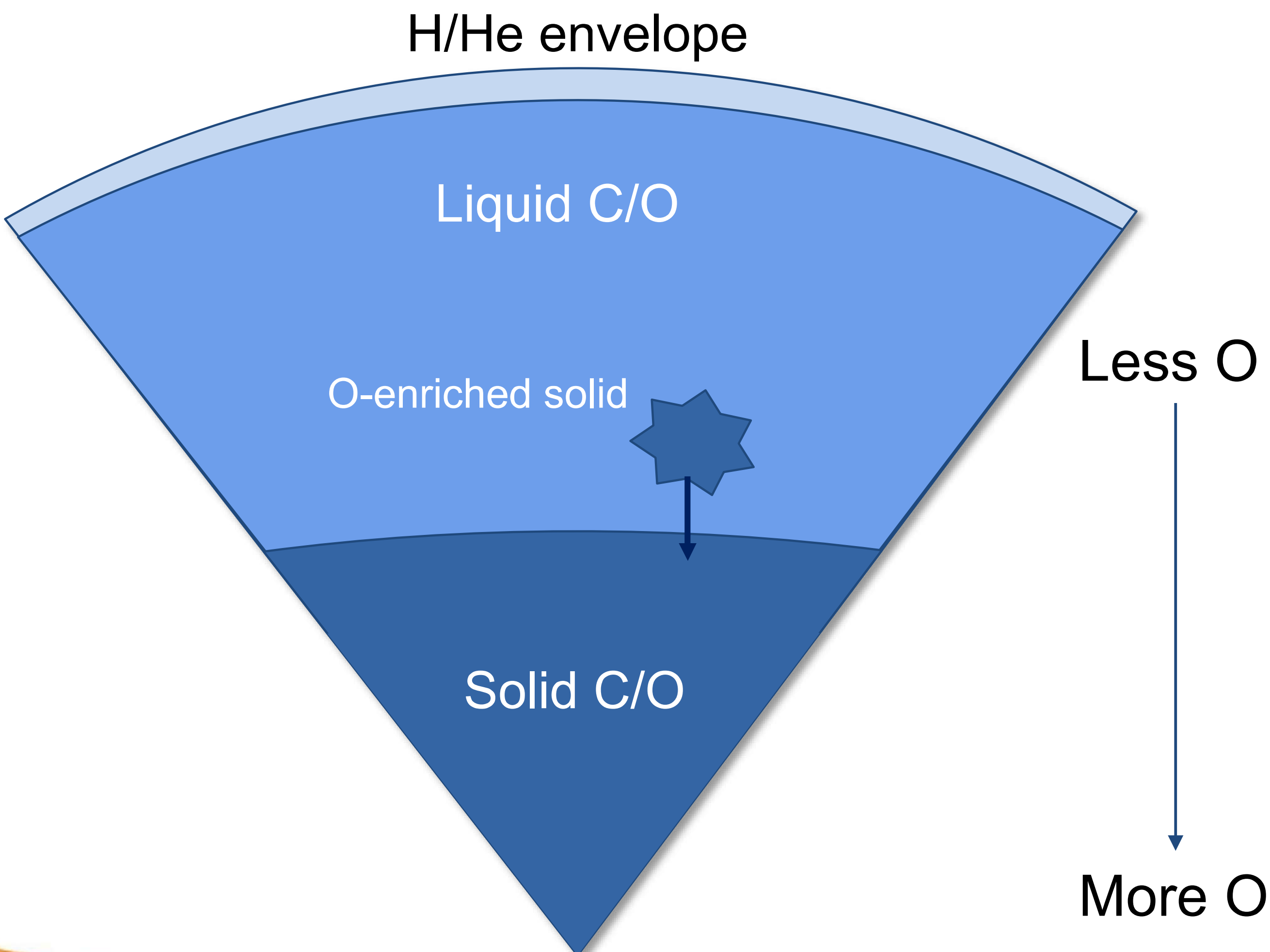
2. Core crystallization



3. Phase diagram calculation

4. C
o

Carbon/oxygen phase separation

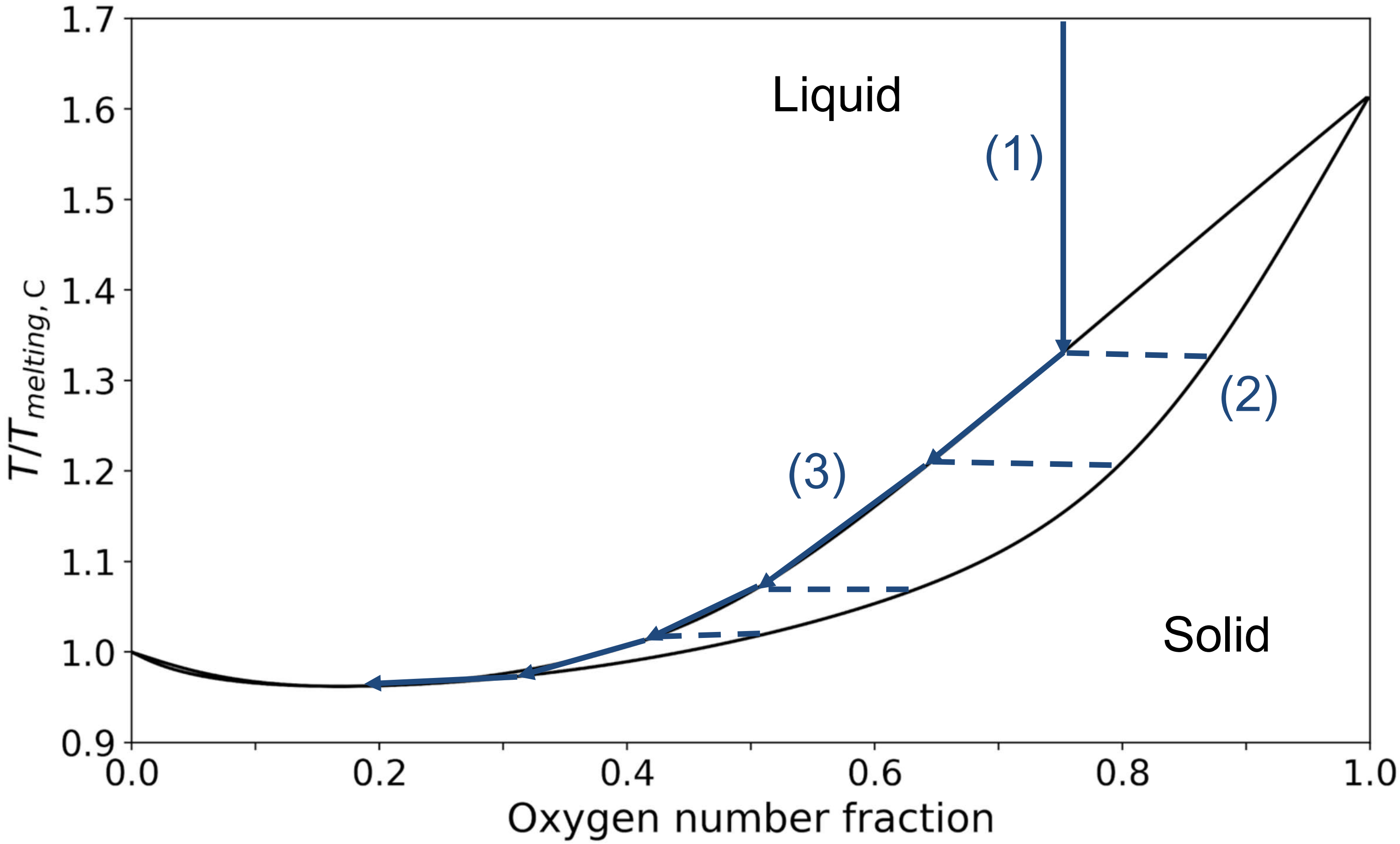


The crystallization fro
upward as the core c

The new crystals form
solid-liquid interface a
compared to the liqui

Gradually, a concentr
is built, thereby releas
gravitational energy

The carbon/oxygen phase diagram

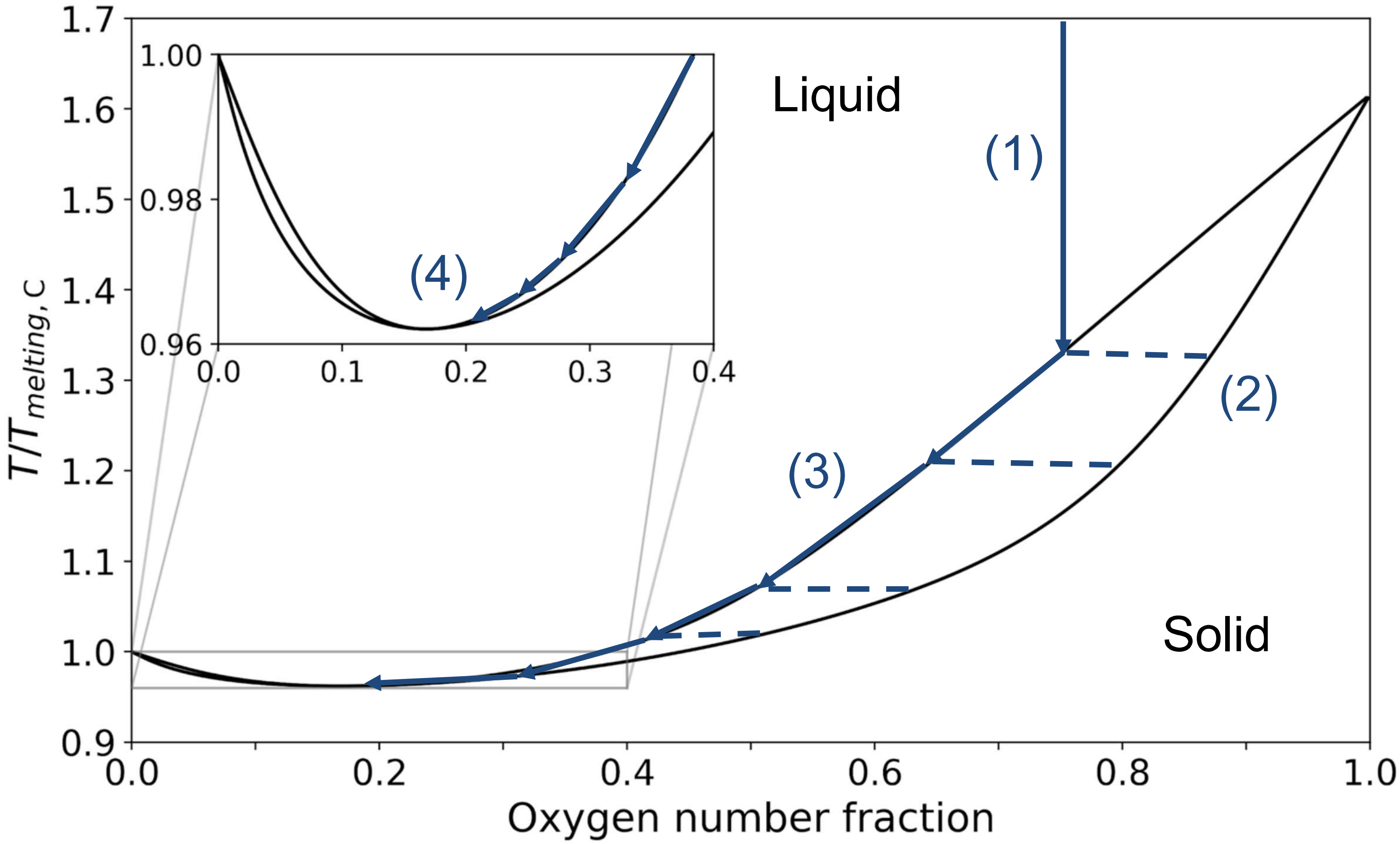


1. The liquid cools
constant concentra
reaches the liquidu

2. The liquid coexi
that contains more

3. As the crystalliz
progresses, the liq
impoverished in O

The carbon/oxygen phase diagram



1. The liquid cools
constant concentra
reaches the liquidu

2. The liquid coexi
that contains more

3. As the crystalliz
progresses, the liq
impoverished in O

4. This process ev
when the azeotrop

Previous attempts at computing the C/O phase dia

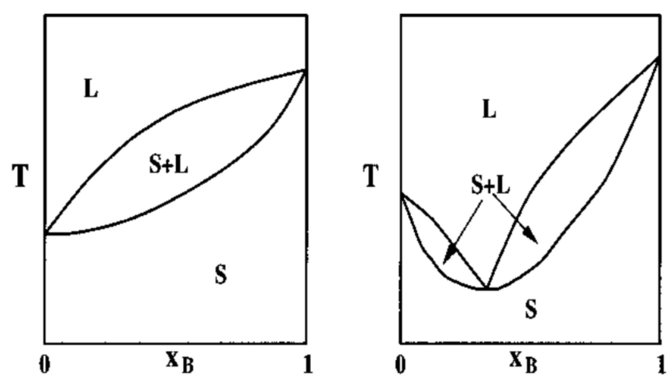
<u>Option 1</u>: Analytical free energy models

Need to interpolate sparse simulation data, so results are sensitive to arbitrary choices made when building the interpolation functions

$$f_{\mathrm{mix}} = x_1 f_{\mathrm{OCP}}(\Gamma_1) + x_2 f_{\mathrm{OCP}}$$

fitted to MC calculation

Even the *qualitative* shape of the phase diagram is affected by those choices (DeWitt et al. 1996)



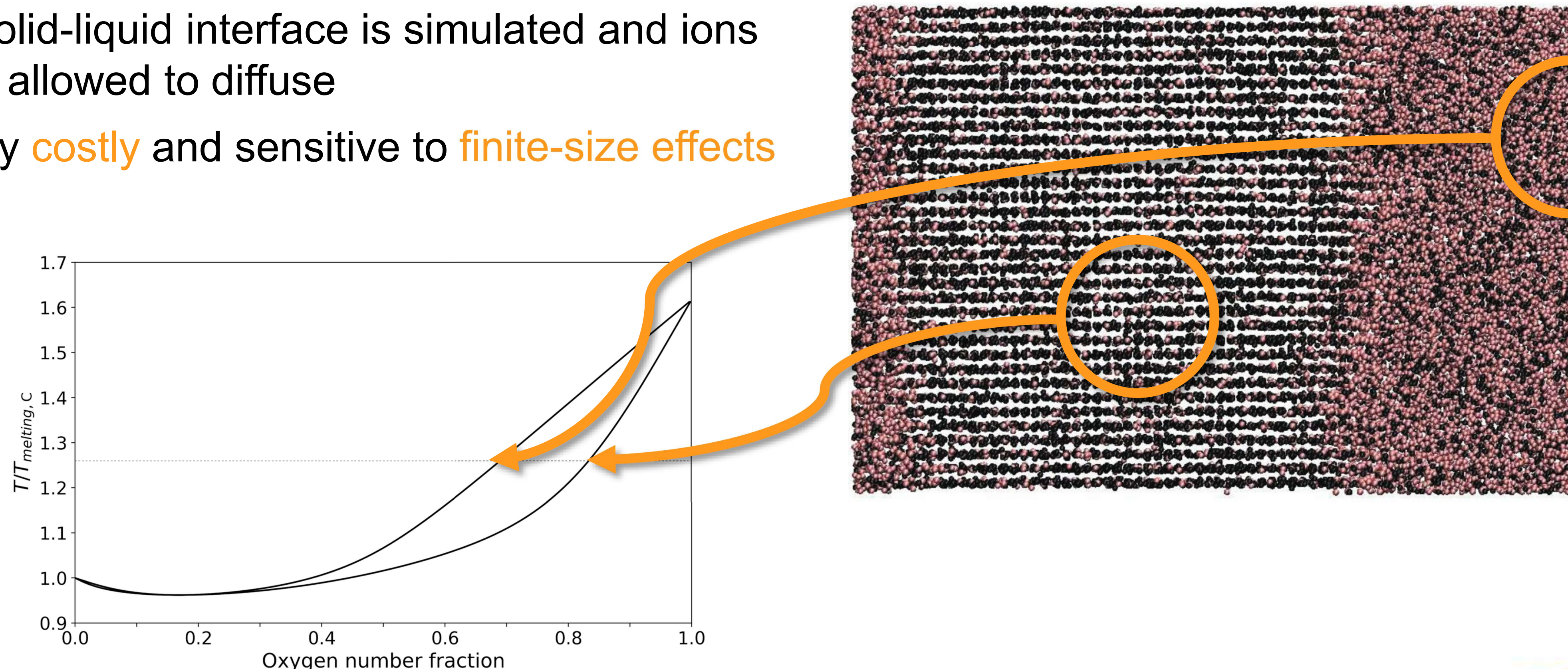
Hitchcock & Hall 1999

Previous attempts at computing the C/O phase dia

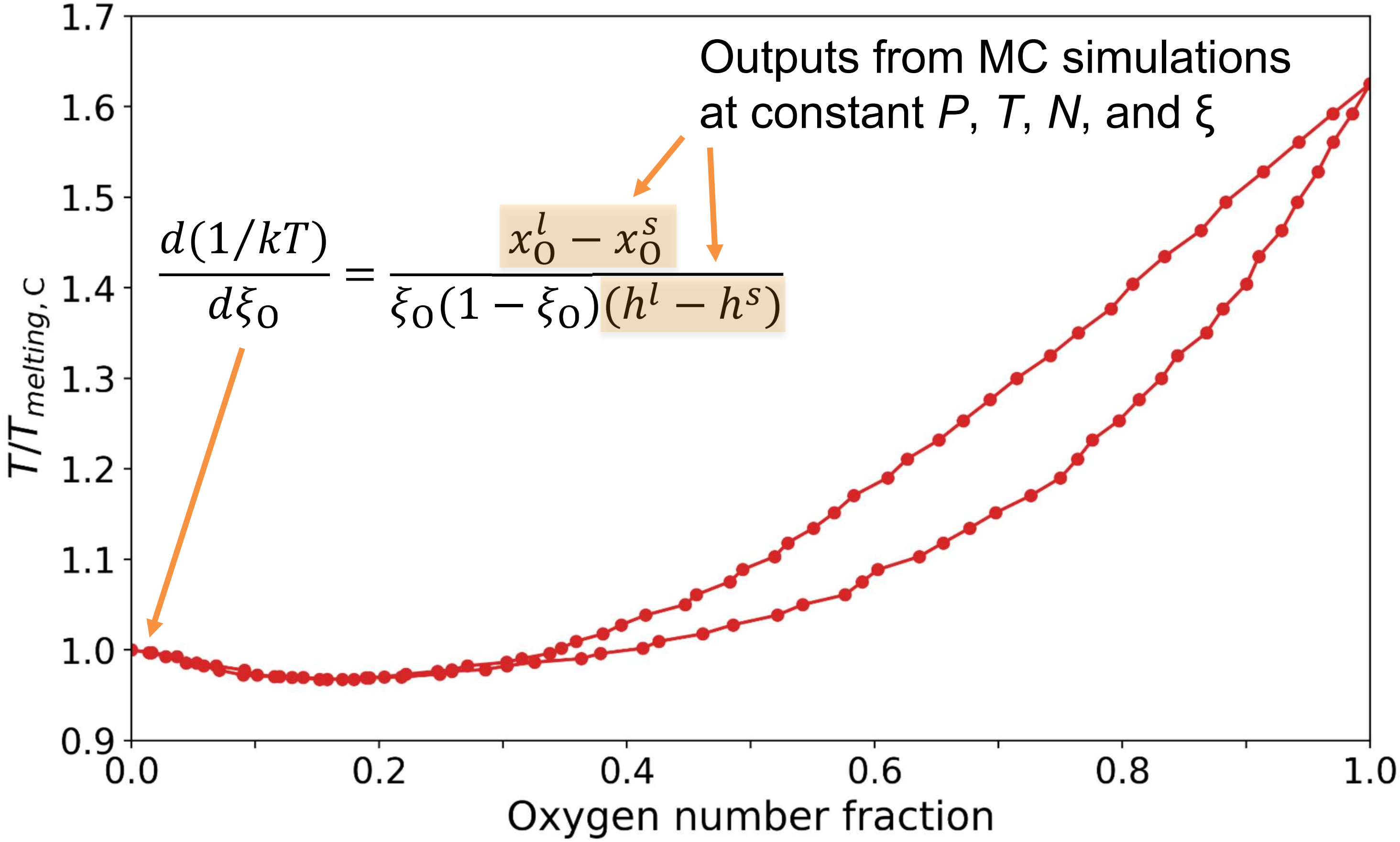
<u>Option 2</u>: Two-phase MD simulations

A solid-liquid interface is simulated and ions are allowed to diffuse

Very costly and sensitive to finite-size effects



The Gibbs-Duhem integration technique



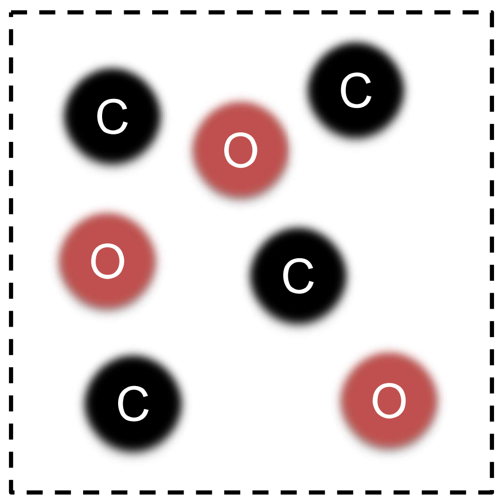
Technique previously
neutral mixtures; we h
to plasmas

Relies on the Monte C
and the Clapeyron equ

$$\frac{dP}{dT} = \frac{\Delta}{\Delta}$$

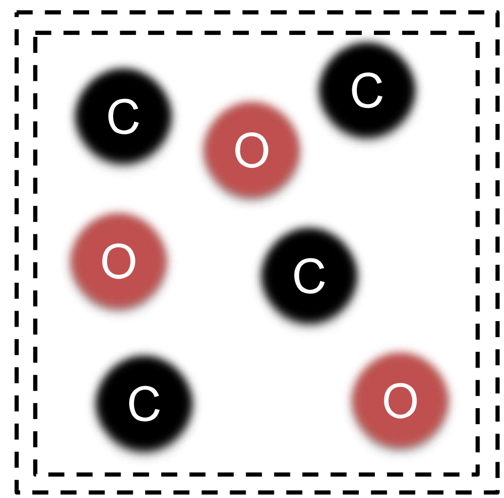
Integration along the li
coexistence curve in th
fugacity space

Semigrand canonical MC simulations

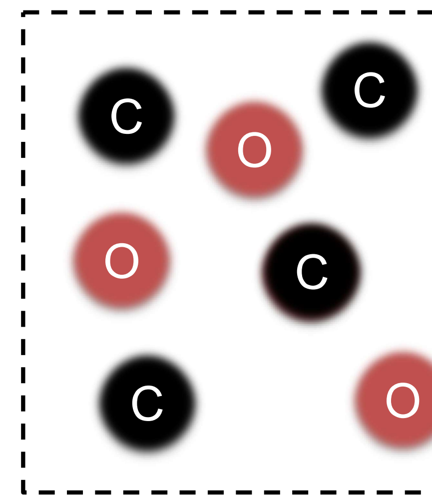


1. Ion displacement

Limited for solid (bcc) phase



2. Volume change



3. Identity chang

The volume and the number of ions of each species are not fixed (but P and N_{tot}

Those steps insure that the energy is minimized and that the targeted pressure a fugacity fraction (ξ_O) are reached

Semigrand canonical MC simulations

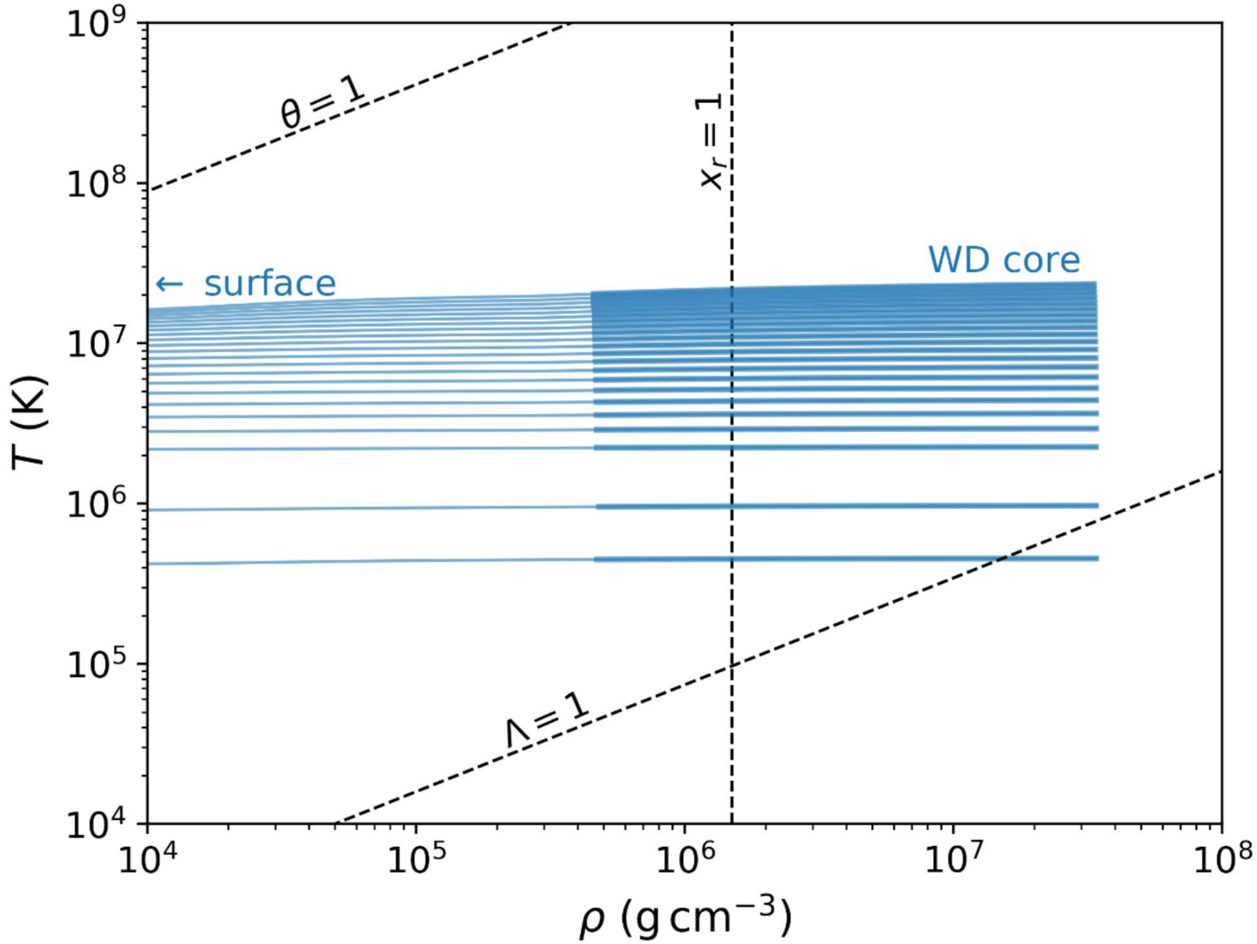
The choice of the type of MC move is randomly chosen at each iteration: particle displacement or volume change or identity change

The overall acceptance probability of a move is $\min(1, e^{\Lambda})$, where

$$\Lambda = -\beta\left(U^{\text{trial}} - U^{\text{old}}\right) - \beta P\left(V^{\text{trial}} - V^{\text{old}}\right) + N \ln \frac{V^{\text{trial}}}{V^{\text{old}}} + m \ln \frac{\xi_0}{1 - \xi_0}$$

$m = \pm 1$

Physics included in our MC simulations



The plasma is completely ioniz

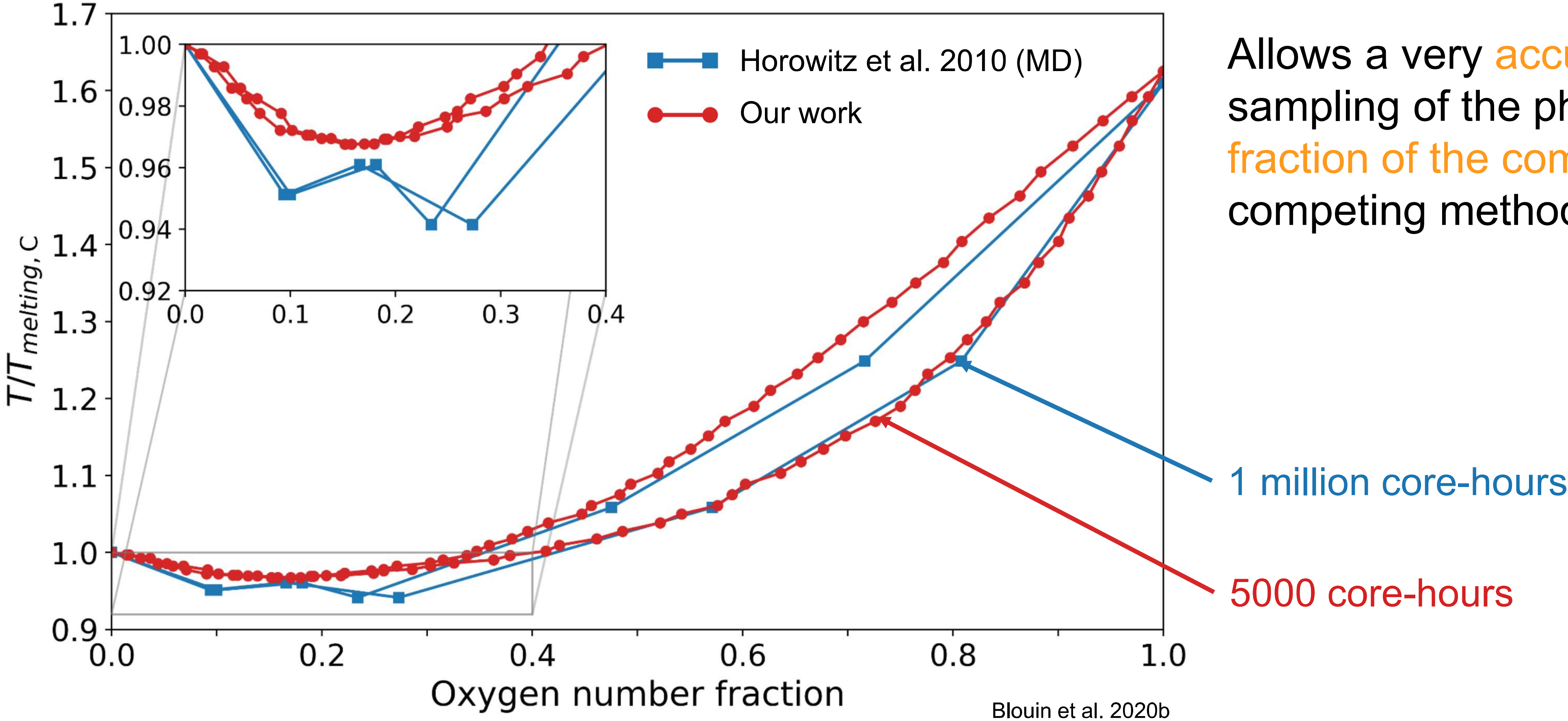
The degenerate, partially relati
jellium is explicitly included in t

The ion-ion interactions are scr
partially relativistic electrons,

$$V(r) = \frac{q^2}{r}\exp(-\kappa r$$

Not included: quantum behavio

Our new C/O phase diagram



Blouin et al. 2020b

Allows a very accurate sampling of the phase fraction of the computa competing methods

Major advantages of the Gibbs-Duhem technique

All calculations are done in the relevant statistical ensemble: phase transitions take place at constant P, not constant V

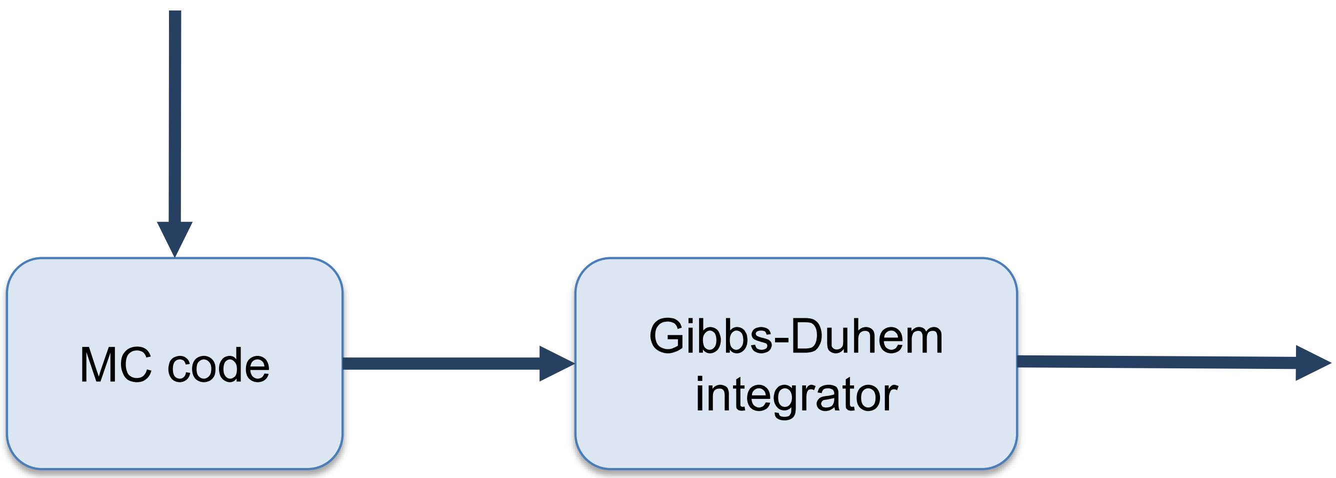
We have access to all thermodynamic properties at the phase transition (e.g., latent heat) at no additional cost (not the case with MD)

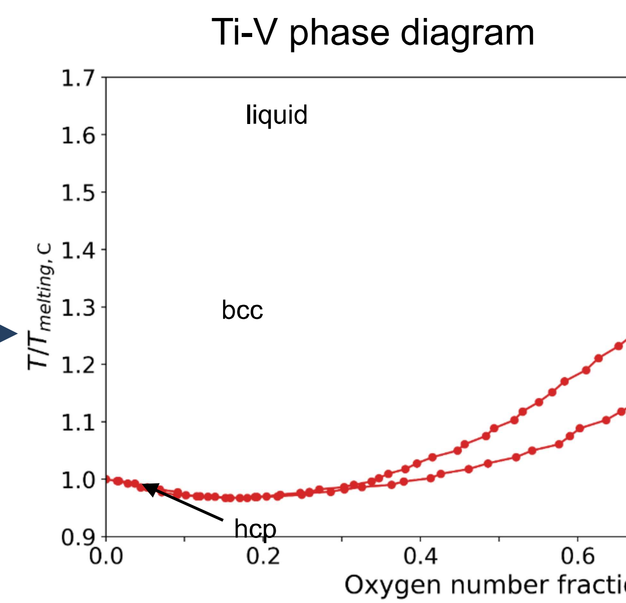
Future applications

This new simulation capability can easily b
obtain phase diagrams of non-astrophysic
(e.g., alloys)

We are working on adding the option of co
phase diagrams for ternary mixtures/alloys

$$V(r) = \frac{q^2}{r} exp(-\kappa r/a)$$



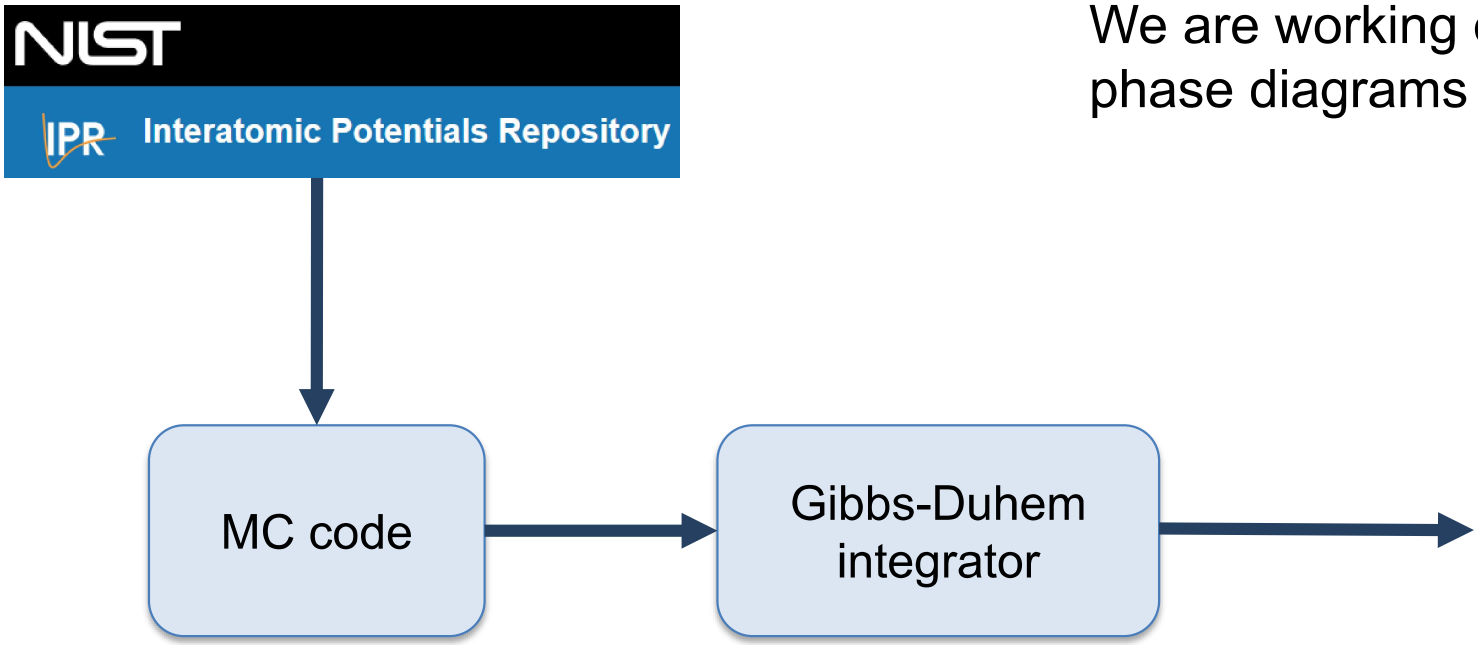


Ghosh 2002

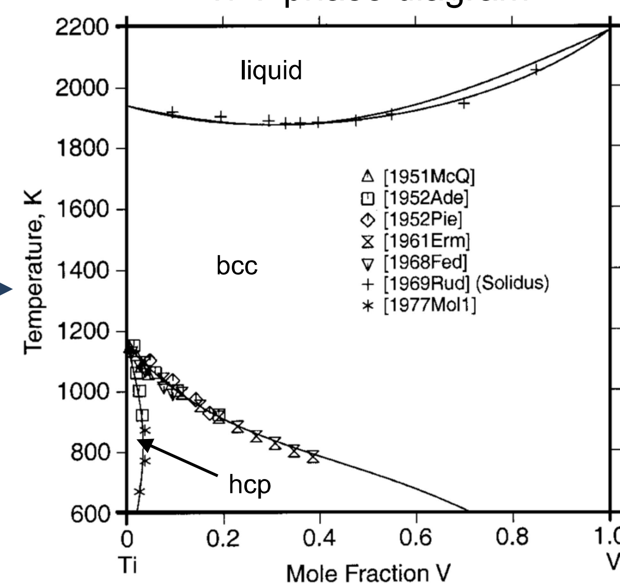
Future applications

This new simulation capability can easily b
obtain phase diagrams of non-astrophysic
(e.g., alloys)

We are working on adding the option of co
phase diagrams for ternary mixtures/alloys

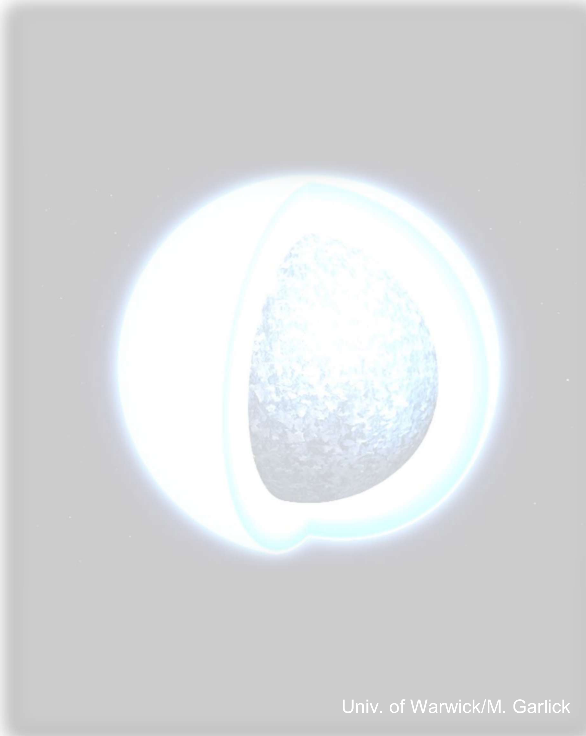


Ti-V phase diagram

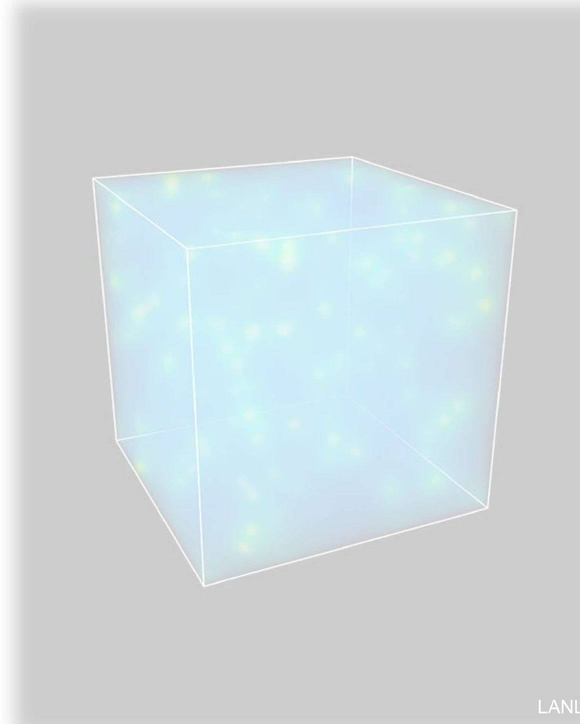


Ghosh 2002

1. What are white dwarfs and why are they interesting?



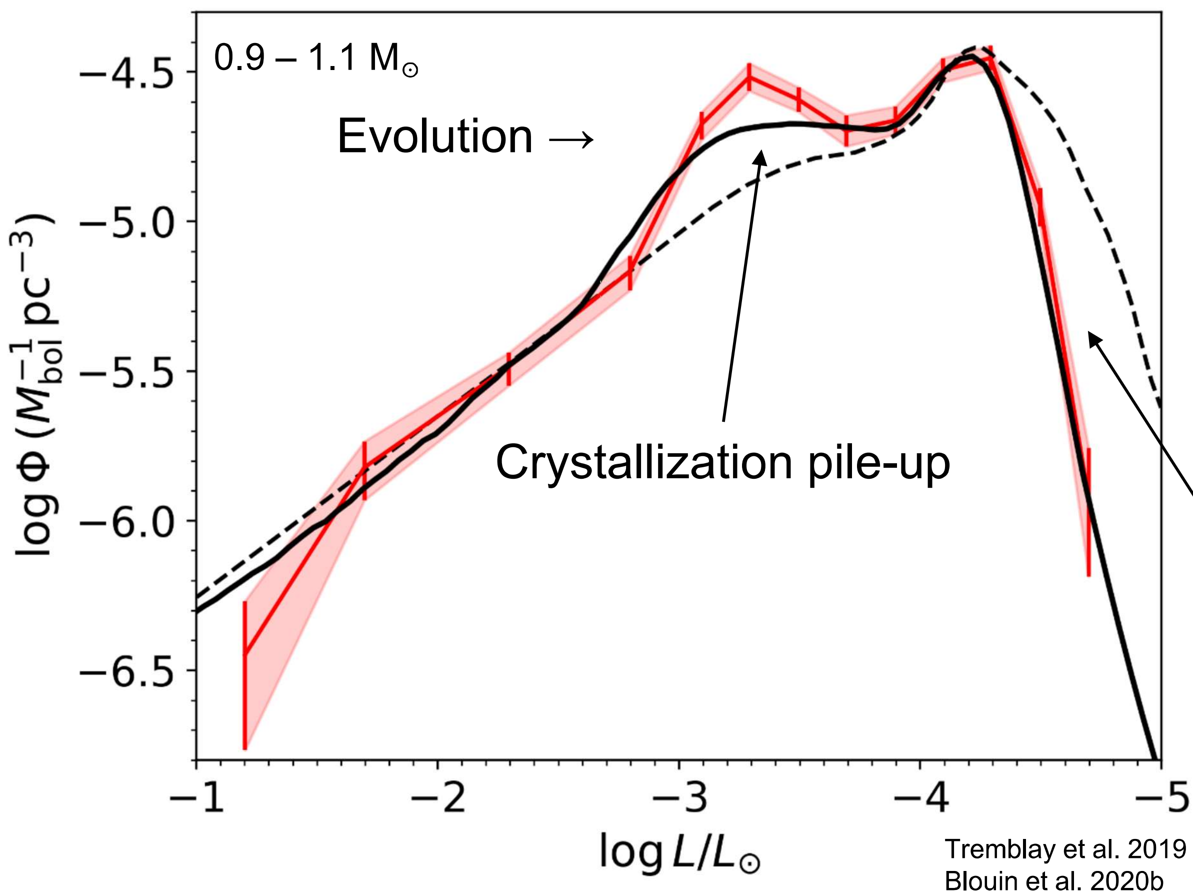
2. Core crystallization



3. Phase diagram calculation

4. C
o

Comparison to observational data



Core crystallization leaves a
on the luminosity function o
WDs, allowing a direct com
observations

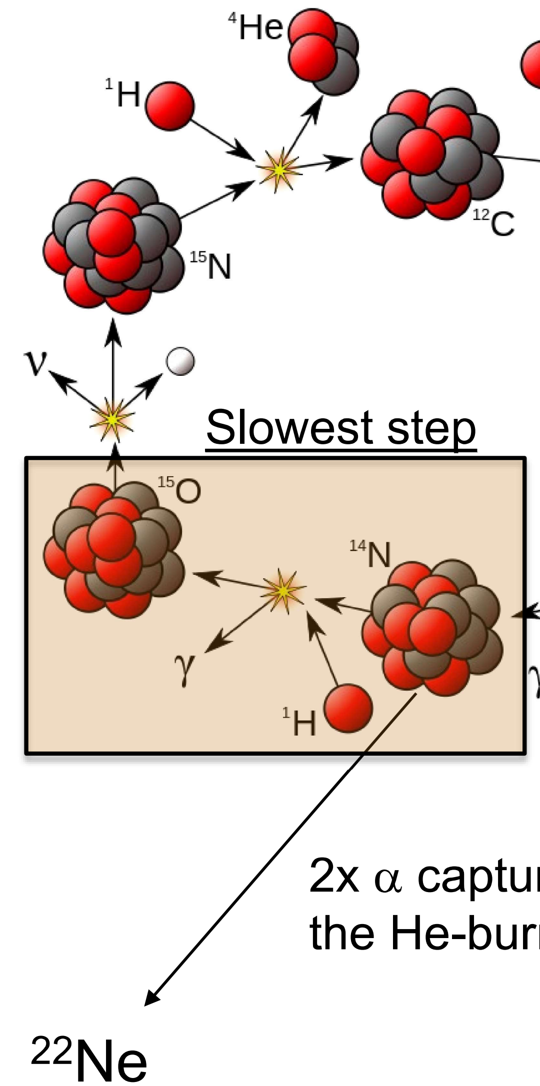
The underestimation of the
crystallization pile-up may b
role of a 3rd minor species,

^{22}Ne in white dwarfs

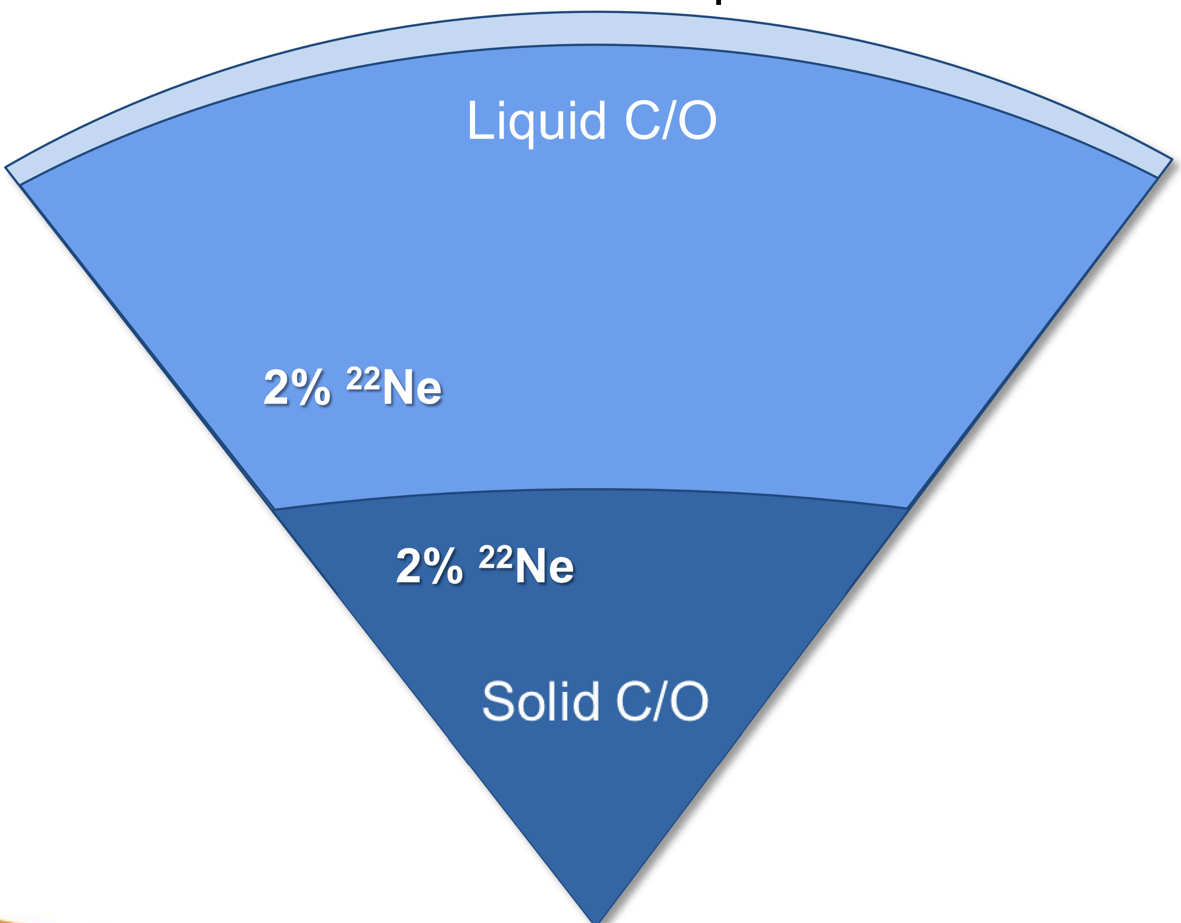
^{22}Ne makes up about 1-2% of a WD's mass

It is produced from the leftovers of the H-burning phase

Because it has 2 excess neutrons (Z=10, A=22), the sedimentation of a given quantity of ^{22}Ne releases ~25 times more gravitational energy than the sedimentation of the same amount of ^{16}O



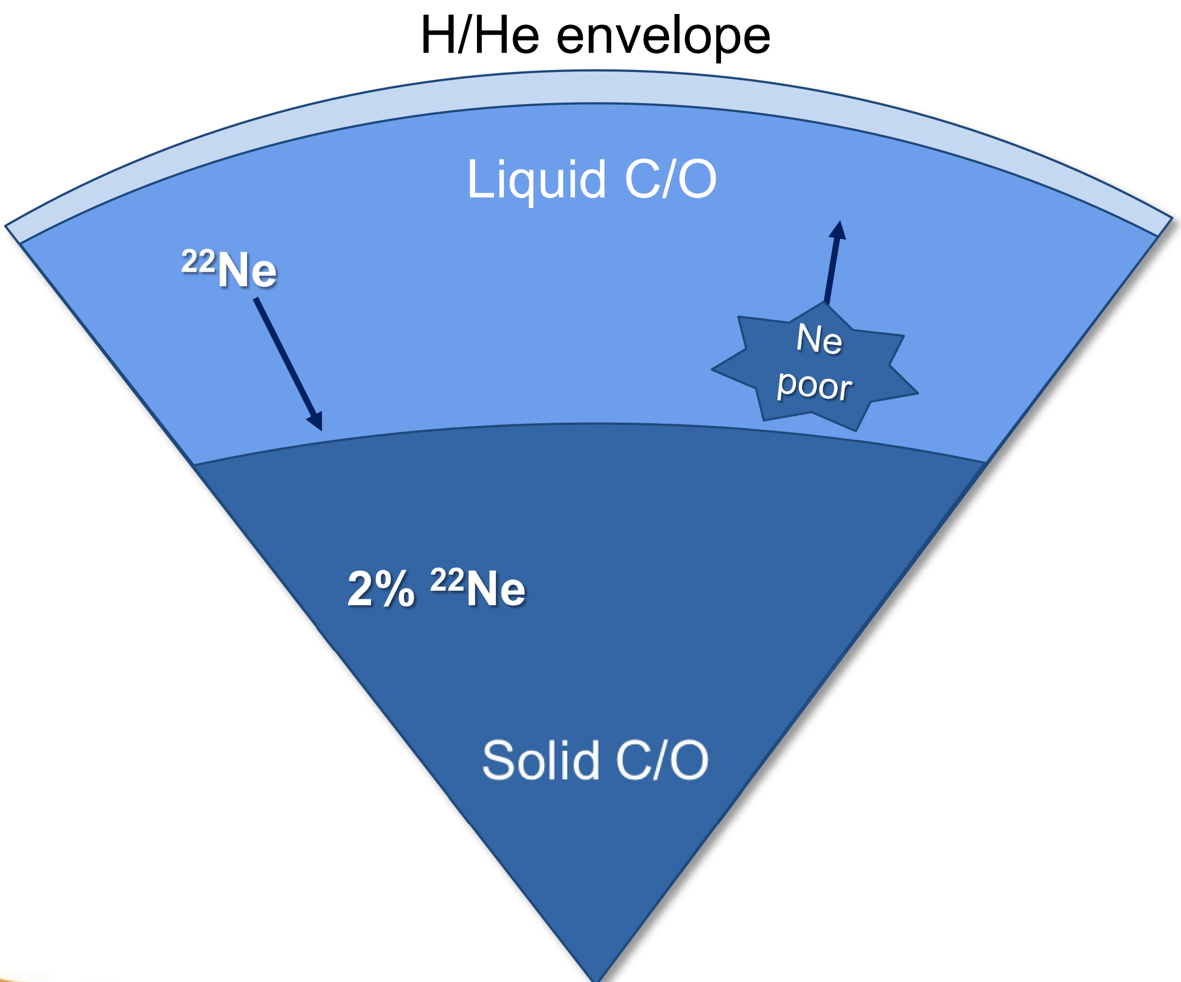
What may be going on with ^{22}Ne



Preliminary calculations of the C
diagram suggest that:

1. At first, there is no ^{22}Ne pha

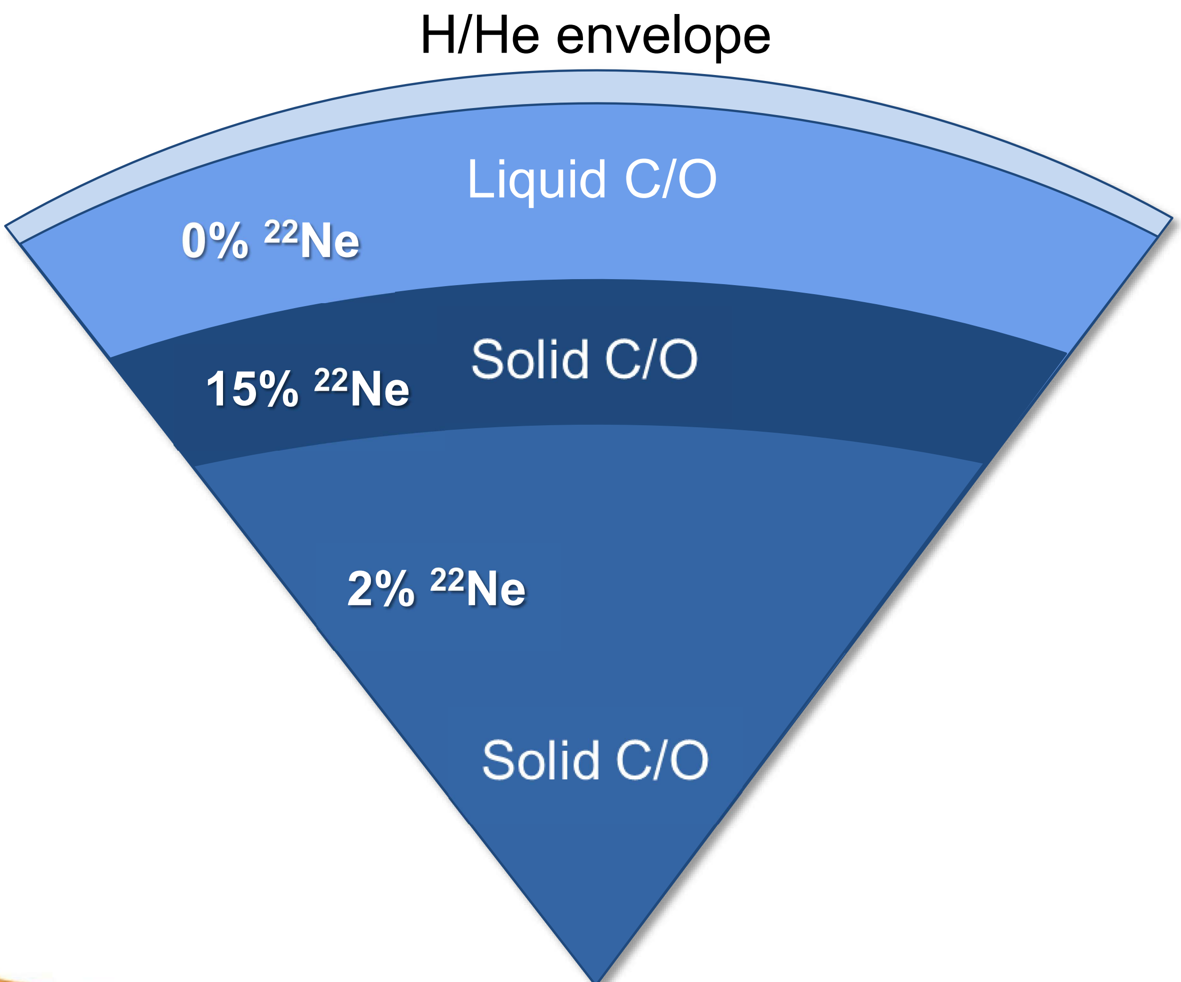
What may be going on with ^{22}Ne



Preliminary calculations of the C
diagram suggest that:

1. At first, there is no ^{22}Ne pha
2. Later, when approaching th azeotrope, the solid is depl compared to the liquid
3. The ^{22}Ne-poor solid floats, ^{22}Ne-rich liquid to the cryst

What may be going on with ^{22}Ne



Preliminary calculations of the (
diagram suggest that:

1. At first, there is no ^{22}Ne pha
2. Later, when approaching th
azeotrope, the solid is depl
compared to the liquid
3. The ^{22}Ne-poor solid floats,
^{22}Ne-rich liquid to the crysta
4. Eventually, the azeotrope is
all the remaining ^{22}Ne is fro
^{22}Ne-rich layer, resulting in
cooling delay

Summary

White dwarfs offer unique opportunities to study the history of our Galaxy

New observational datasets challenge our understanding of white dwarfs and call for refined physics models

We have developed an efficient and physically accurate technique to model the phase transition undergone by white dwarfs

This new technique can now be applied to other systems

Thank you! Questions?