VICE: Versatile Integrator for Chemical Evolution

Science Documentation

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1) Introduction

VICE concerns itself with galactic chemical evolution (GCE) modeling, operating under the single-zone approximation. This is also known to as the one-zone approximation, and the associated physical models are sometimes referred as "box models." Box models by design do not track phase-space information for discrete gas and star particles, and they thus fail to capture dynamical effects which can influence galactic chemical abundance patterns, such as the radial migration of stars. Nonetheless, box models still have the capability of capturing the highly nonlinear physics associated with GCE, such as the nucleosynthetic yields of various elements from different types of supernovae (e.g. Woosley & Weaver, 1995; Iwamoto et al., 1999; Chieffi & Limongi, 2004, 2013; Limongi & Chieffi, 2018) and asymptotic giant branch stars (e.g. Karakas, 2010; Cristallo et al., 2011), the dependence of star formation efficiency on the density of interstellar gas (e.g. Schmidt, 1959; Kennicutt, 1998; Leroy et al., 2008), and arbitrary infall and star formation histories which vary from galaxy to galaxy. By not tracking phase-space information, box models assume a uniform gas density and spatially uniform star formation efficiency, as well as instantaneous mixing of metals in the interstellar medium (ISM). The addition of phase-space information, while capturing dynamical effects which influence galaxies, require N-body or hydrodynamic treatments. These simulations are highly computationally expensive, often requiring thousands of computing hours. The assumption of spatial homogeneity reduces GCE models to a system of coupled integro-differential equations with time - a drastic reduction in computational expense from a full N-body treatment. What box models lose in the assumption of spatial homogeneity they more than make up for in computational expense.

2) Implementation

As discussed in section 1, the assumption of spatial homogeneity reduces the highly nonlinear mathematics of GCE modeling to a system of coupled integro-differential equations of time. While this is still a highly nonlinear set of equations and thus a tremendously difficult problem analytically, given the boundary conditions, the initial value problem can be integrated numerically with minimal computational expense. In this section we detail the equations of single-zone enrichment as they are implemented in VICE. We simultaneously present the numerical approximations adopted by the algorithm, which constitute a timestep-style method using Euler's method (Numerical Recipes Ch. XX). We acknowledge that of the most common numerical integration techniques, Euler's method has the largest numerical errors. However, the assumption of spatial homogeneity introduces errors at the ~few% level in comparison to observations even for the best of fits (citation). Knots in the density field and diffusion timescales of metals in the ISM gas introduce physical scatter about the predictions of box models; they implicitly predict trends in the mean chemical abundance patterns in galaxies. Euler's method thus suffices for our purposes, because the errors introduced by the integration are much smaller than the errors intrinsically associated with the models.

We will also see that as an unintended but beneficial side effect, Euler's method allows us to model each timestep as a single episode of star formation. We determine the time-dependent enrichment for an arbitrary element from core collapse supernovae (CCSNe), type Ia supernovae (SNe Ia), and asymptotic giant branch (AGB) stars. At each timestep, we then take advantage of single stellar populations and simply add up the contributions to each element from all previous timesteps. With integration functions written purely in ANSI/ISO C, this allows VICE to achieve powerful computing speeds. With timesteps of Δt = 1, 10, and 50 Myr (a relatively fine, standard, and coarse timestep), a simulation of 10 billion years of galactic chemical enrichment runs in 6.53 s, 89.7 ms, and 22.5 ms per simulated element, respectively.

3) The Gas Supply

Here we detail the analytic expressions quantifying the amount of gas in a galaxy as a function of time. For a spatially homogeneous cloud of gas with mass infall rate (IFR) $\dot{M}_{\rm in}$, star formation rate (SFR) $\dot{M}_*$, and outflow rate (OFR) $\dot{M}_{\rm out}$, the time-derivative of the mass of the ISM gas is given by:

$$\dot{M}_{\rm g} = \dot{M}_{\rm in} - \dot{M}_* - \dot{M}_{\rm out} + \dot{M}_{\rm r} \tag{1a}$$

$$\approx \dot{M}_{\rm in} - \dot{M}_*(1 + \eta - r_{\rm inst}) \tag{1b}$$

$$= \dot{M}_{\rm in} - M_{\rm g}\tau_*^{-1}(1 + \eta - r_{\rm inst}) \tag{1c}$$

where $\dot{M}_{\rm returned}$ quantifies the amount of gas returned to the ISM by stars as the various channels of stellar death. Here we have made use of the commonly applied approximations $\dot{M}_{\rm out} \approx \eta\dot{M}_*$ and $\dot{M}_{\rm returned} \approx r_{\rm inst}\dot{M}_*$ (e.g. Weinberg et al., 2017, hereafter WAF17), where η is known as the *mass loading factor* and $r_{\rm inst}$ is an instantaneous recycling parameter. We have also made the substitution $\dot{M}_* \equiv M_{\rm g}\tau_*$, the definition of the star formation efficiency (SFE) timescale τ_*. We note that this quantity is more conventionally referred to as the *depletion time*; WAF17 used a redefinition of the depletion time $\tau_{\rm dep} \equiv M_{\rm g}/(\dot{M}_* + \dot{M}_{\rm out} - \dot{M}_{\rm returned}) \approx \tau_*/(1 + \eta - r_{\rm inst})$ to reflect that the depletion time is also affected by outflows and recycling, and we retain this nomenclature here, referring to τ_* as the SFE timescale.

Numerically, equation 1a is implemented in the following manner:

$$\Delta M_{\rm g} \approx \dot{M}_{\rm in}\Delta t - \dot{M}_*\Delta t - \dot{M}_{\rm out}\Delta t + \Delta M_{\rm returned} \tag{2}$$

where the star formation rate and gas supply are related by the definition of the SFE timescale ($\tau_* \equiv M_{\rm g}/\dot{M}_*$). By design, the `integrator` operates in `ifr` mode, meaning that the user has specified an infall history as a function of time. This can be switched to either `sfr` or `gas` if the user would like to specify a star formation history or a gas history, respectively. The treatment of outflows and recycling in `VICE` is not mathematically trivial, so we leave their details to subsequent sections. With this information, the solution to equation 2 is unique.

3.1) Outlows

The conventionally adopted relation between the outflow and star formation rates is given by $\dot{M}_{\rm out} = \eta\dot{M}_*$. In `VICE` we introduce a new parameter into single-zone models which we dub the *smoothing time*, which attempts to generalize this relation beyond its current state:

$$\dot{M}_{\rm out} = \eta(t)\langle\dot{M}_*(t)\rangle_{\tau_{\rm s}} \tag{3}$$

The smoothing time denotes the timescale on which the star formation rate is averaged, before it is then multiplied by the mass loading factor η to determine the mass outflow rate. This prescription for outflow rates has the following analytic form:

$$\dot{M}_{\rm out} = \begin{cases} \dfrac{\eta(t)}{\tau_s}\displaystyle\int_{t-\tau_{\rm s}}^{t} \dot{M}_*(t')dt' & (t \geq \tau_{\rm s}) \\ \dfrac{\eta(t)}{t}\displaystyle\int_0^t \dot{M}_*(t')dt' & (0 \leq t \leq \tau_{\rm s}) \end{cases} \tag{4a}$$

$$\rightarrow \begin{cases} \eta(t)\dfrac{\Delta t}{\tau_{\rm s}}\displaystyle\sum_{i=0}^{\tau_{\rm s}/\Delta t} \dot{M}_*(t - i\Delta t) & (t \geq \tau_{\rm s}) \\ \eta(t)\dfrac{\Delta t}{t}\displaystyle\sum_{i=0}^{t/\Delta t} \dot{M}_*(t - i\Delta t) & (0 \leq t \leq \tau_{\rm s}) \end{cases} \tag{4b}$$

where the $\rightarrow$ denotes the switch from the analytic treatment to the numerical approximation adopted by `VICE`. In words, at each timestep `VICE` simply looks back the number of timesteps corresponding to the smoothing time, and determines the arithmetic mean of the star formation rate over those timesteps. An advantage of this formulation is that when $\tau_{\rm s} < \Delta t$, `VICE` recovers the traditional relation $\dot{M}_{\rm out} = \eta(t)\dot{M}_*(t)$ automatically.

The mass-loading parameter is a user-specified function of time. By implementing the mass loading factor in this manner, `VICE` achieves the capability of simulating galaxies with arbitrarily complex mass loading factors. We clarify that it is only the star formation rate which is time-averaged under this formulation; the user-specified $\eta(t)$ is taken to be an instantaneous function.

3.2) Recycling

As stars evolve off the main sequence, leaving behind a remnant, whatever mass does not end up in the remnant is returned to the ISM. Here we define the *cumulative return fraction* (CRF) $r(t)$ as the fraction of a single stellar population's mass which is returned to the ISM at a time t following its formation. This parameter is specified by the adopted IMF, the lifetimes of stars on the main sequence as a function of mass, and the mass of stellar remnants left behind also as a function of mass. Given the cumulative return fraction $r(t)$, the rate of gas return via this channel is given by:

$$\dot{M}_{\rm returned} = \int_0^t \dot{M}_*(t-t')\frac{dr(t')}{dt}dt \tag{5a}$$

$$\rightarrow \sum_{i=0}^{t/\Delta t} \dot{M}_*(t-i\Delta t)[r((i+1)\Delta t) - r(i\Delta t)] \tag{5b}$$

where the $\rightarrow$ again denotes the switch from the analytic expression to the numerical approximation implemented in `VICE`.

`VICE` adopts the approximation that the post-mainsequence lifetimes of stars are short (i.e. instantaneous), and so as stellar populations evolve off the main sequence, they are treated as if they instantaneously produce a remnant and return a given amount of gas to the ISM. We adopt the common approximation for the main-sequence lifetimes of stars:

$$\tau_{\rm MS} \approx \tau_{\rm MS}^{\odot}\left(\frac{M}{M_\odot}\right)^{-3.5} \tag{6}$$

This implies a main sequence turnoff mass at a time t given by:

$$M_{\rm to} = M_\odot\left(\frac{t}{\tau_{\rm MS}^{\odot}}\right)^{-1/3.5} \tag{7}$$

where we adopt $\tau_{\rm MS}^{\odot} = 10$ Gyr as the main sequence lifetime of the sun. While this is a poor approximation for massive stars ($M \gtrsim 8M_\odot$), these stars have short lifetimes (~few Myr) compared to the relevant timescales for GCE (~few Gyr). For this reason, recycling is fast immediately following a single stellar population's formation anyway. The long-term recycling behavior in galaxies is dominated by stars that return gas to the ISM on timescales closer to 1 Gyr.

Aside from an IMF, this is one of the two pieces of information required to calculate the CRF. The second is the mass of remnants left behind at an initial stellar mass M. We adopt the following model of remnant masses from Kalirai et al. (2008):

$$M_{\rm rem} = \begin{cases} 1.44M_\odot & (M \geq 8M_\odot) \\ 0.394M_\odot + 0.109M & (M < 8M_\odot) \end{cases} \tag{8}$$

Given this information and an adopted IMF dN/dm, the CRF has the following analytic form:

$$r(t) = \int_{m_{\rm to}(t)}^{u} (m - m_{\rm rem})\frac{dN}{dm}dm\left[\int_l^u m\frac{dN}{dm}dm\right]^{-1} \tag{9}$$

where we adopt the nomenclature $m = M/M_\odot$, and u and l denote the upper and lower mass limits on star formation divided by the mass of the sun. Equation 9 is simply the total mass of stars above the turnoff mass minus their remnant masses divided by the total mass of the stellar population. Adopting a power-law IMF $dN/dm = \beta m^{-\alpha}$ and zooming

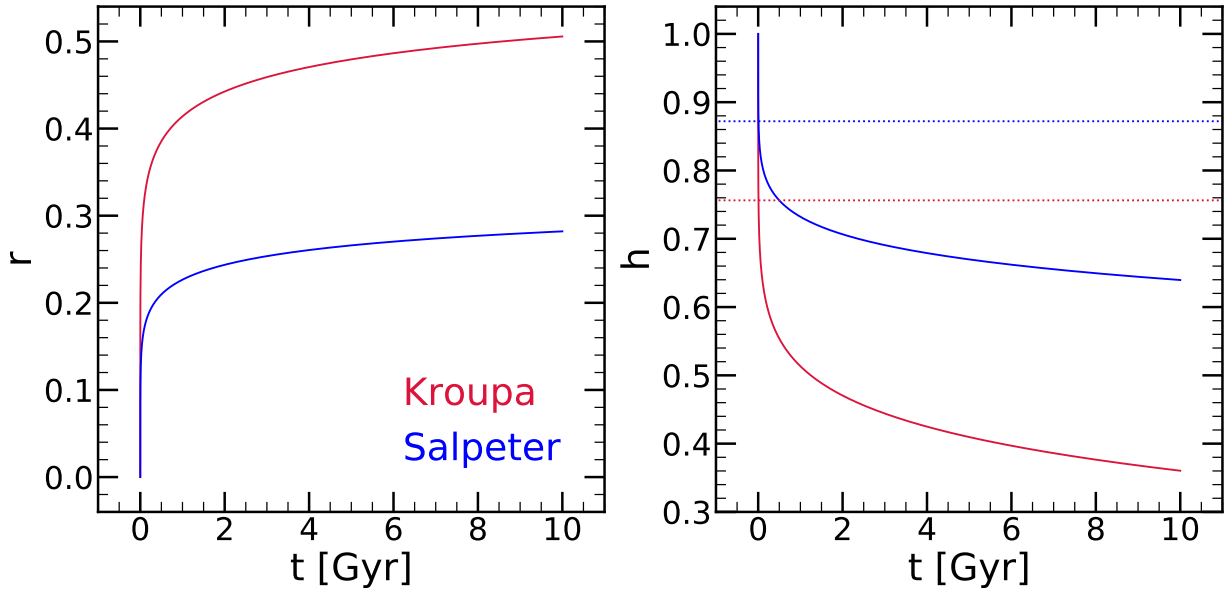

Figure 1: **Left**: The cumulative return fraction r for a single stellar population as a function of time for both Kroupa (red) and Salpter (blue) initial mass functions (Kroupa, 2001; Salpeter, 1955).

in on the numerator:

$$\begin{aligned}
\int_{m_{\rm to}(t)}^{u} (m - m_{\rm rem})\beta m^{-\alpha} dm &= \int_{m_{\rm to}(t)}^{u} \beta m^{1-\alpha} dm - \int_{m_{\rm to}(t)}^{u} \beta m_{\rm rem} m^{-\alpha} dm \\
&= \frac{\beta}{2-\alpha} m^{2-\alpha}\Big|_{m_{\rm to}(t)}^{u} - \begin{cases} \displaystyle\int_{m_{\rm to}(t)}^{u} 1.44\beta m^{-\alpha} dm & (m_{\rm to}(t) \geq 8) \\ \displaystyle\int_{8}^{u} 1.44\beta m^{-\alpha} dm + \int_{m_{\rm to}(t)}^{8} (0.394 + 0.109m)\beta m^{-\alpha} & (m_{\rm to}(t) < 8) \end{cases} \\
&= \frac{\beta}{2-\alpha} m^{2-\alpha}\Big|_{m_{\rm to}(t)}^{u} - \begin{cases} \displaystyle\frac{1.44\beta}{1-\alpha} m^{1-\alpha}\Big|_{m_{\rm to}(t)}^{u} & (m_{\rm to}(t) \geq 8) \\ \displaystyle\frac{1.44\beta}{1-\alpha} m^{1-\alpha}\Big|_{8}^{u} + \left[\frac{0.394\beta}{1-\alpha} m^{1-\alpha} + \frac{0.109\beta}{2-\alpha} m^{2-\alpha}\right]_{m_{\rm to}(t)}^{8} & (m_{\rm to}(t) < 8) \end{cases}
\end{aligned} \tag{10}$$

For piece-wise IMFs like Kroupa (2001), this simply becomes a summation over the different mass ranges with different power law indeces. The denominator of $r(t)$ is simply the total mass of the stellar population:

$$\int_{l}^{u} \beta m^{1-\alpha} dm = \frac{\beta}{2-\alpha} m^{2-\alpha}\Big|_{l}^{u} \tag{11}$$

It is the analytically integrated forms of equations 10 and 11 which we have built into `VICE`; this reduces computational expense by eliminating the requirement for built-in numerical quadrature functions. At the beginning of each simulation, `VICE` simply samples $r(t)$ at all timesteps and stores its value at each Δt interval in time, then evaluating equation 5b from each previous episode of star formation.

With a user-specified infall history, star formation history, or gas supply history, the outflow prescription outlined in section 3.1, and `VICE`'s recycling implementation in section 3.2, the numerical soluation to equation 2 is unique. This is how `VICE` determines the change in gas supply at each timestep.

4) Enrichment

In this section we present the equations detailing the time-dependent enrichment of a given element in the single-zone approximation and how they are implemented numerically in `VICE`. The time-derivative of the total mass of an element x is given by:

$$\dot{M}_{\rm x} = \dot{M}_{\rm x}^{\rm CC} + \dot{M}_{\rm x}^{\rm Ia} + \dot{M}_{\rm x}^{\rm AGB} - \frac{M_{\rm x}}{M_{\rm g}}[\dot{M}_* + \xi_{\rm enh}\dot{M}_{\rm out}] + \dot{M}_{\rm returned} + Z_{\rm x,in}\dot{M}_{\rm in} \tag{12}$$

This equation is simply a mathematical statement of the source and sink terms of a given element in the ISM. At any given time, an arbitrary element will have a given emount of enrichment from core collapse supernovae [$\dot{M}_{\rm x}^{\rm CC}$], type Ia supernovae [$\dot{M}_{\rm x}^{\rm Ia}$], and AGB stars [$\dot{M}_{\rm x}^{\rm AGB}$]. At the same time, it is depleted from the ISM as stars are formed at its metallicity [$(M_{\rm x}/M_{\rm g})\dot{M}_*$] and ejected in outflows at some multiplicative factor of the ISM metallicity [$(M_{\rm x}/M_{\rm g})\dot{M}_{\rm out}\xi_{\rm enh}$]. It is also returned to the ISM as previous generations of stars evolve off the main sequence and return gas to the ISM at their birth metallicity [$\dot{M}_{\rm returned}$]. If there is an inflow with nonzero metallicity, this also adds mass to the ISM [$Z_{\rm x,in}\dot{M}_{\rm in}$]. `VICE` implements the simplest approximation:

$$\Delta M_{\rm x} = \dot{M}_{\rm x}^{\rm CC}\Delta t + \dot{M}_{\rm x}^{\rm Ia}\Delta t + \dot{M}_{\rm x}^{\rm AGB}\Delta t - \frac{M_{\rm x}}{M_{\rm g}}[\dot{M}_* + \xi_{\rm enh}\dot{M}_{\rm out}]\Delta t + \Delta M_{\rm returned} + Z_{\rm x,in}(t)\dot{M}_{\rm in}\Delta t \tag{13}$$

The user has a large degree of customizability over every term on the right-hand side of this equation in `VICE`. We detail the treatment of each term individually.

In this section we do not detail the mathematical formalism of the nucleosynthetic yields from the various channels. We reserve this discussion for section 5.

4.1) Core Collapse Supernovae

Core collapse supernovae (CCSNe) are the thermonuclear detonations of massive stars ($\gtrsim 8M_\odot$) at the end of their lifetimes. These stars live on extremely short timescales (~few Myr) compared to the relevant timescales for galaxy evolution (~few Gyr). Thus it is an excellent approximation to treat the CCSNe associated with an episode of star formation and their ensuing metal enrichment as instantaneous. This implies a direct linear relationship between the core-collapse production and the star formation rate:

$$\dot{M}_{\rm x}^{\rm CC} = y_{\rm x}^{\rm CC}(Z)\dot{M}_* \tag{14}$$

where $y_{\rm x}^{\rm CC}$ is the IMF-integrated core-collapse yield. This is the fraction of an entire stellar population's initial mass which is converted to an element x at a metallicity $Z = M_{\rm x}/M_{\rm g}$.

$$y_{\rm x}^{\rm CC}(Z) = \frac{\int_8^u M_{\rm x}\frac{dN}{dM}dM}{\int_l^u M\frac{dN}{dM}dM} \tag{15}$$

where $M_{\rm x}$ is the mass of element x that is produced on average in the CCSN of a star with initial mass M. The bounds of the integral in the numerator are from 8 to u, because `VICE` operates under the assumption that only $> 8\ M_\odot$ stars explode as CCSNe. The denominator is simply the total mass of stars in a single stellar population.

`VICE` allows the user to specify any functional form for $y_{\rm x}^{\rm CC}(Z)$. It achieves this by sampling their functional yield at every 10^{-5} interval steps in Z between $Z = 0$ and $Z = 0.5$, interpolating on the finely sampled grid at each timestep. This spans the range of physically realistic values in Z. With the star formation rate defined as a function of time either by user specification or by the relations outlined in section 3, the solution to equation 14 is unique. Due to the approximation of instantaneous detonation of core-collapse supernovae, equation 14 is perhaps the simplest relation implemented in `VICE`.

4.2) Type Ia Supernovae

Type Ia supernovae (SNe Ia) are the thermonuclear detonations of white dwarf stars when they reach the Chandrasekhar limit ($\sim 1.4M_\odot$). White dwarves (WDs) associated with a given stellar population (or associated time step in `VICE`) are formed from low-mass stars, and thus take a minimum amount of time to form. It isn't until after a single stellar population forms WDs that SNe Ia will detonate, enriching the ISM with heavy elements.

In order to model the time-dependent enrichment of an element x by SNe Ia, we employ a *delay-time distribution* (DTD) denoted by $R_{\rm Ia}(t)$. This denotes the rate of SNe Ia associated with a single generation of stars at a time t

following its formation, and thus has units of yr^{-1}. Then, at any given timestep, the rate of enrichment of elements x is given by the star formation history weighted by the DTD up to a fractional yield:

$$\dot{M}_{\mathrm{x}}^{\mathrm{Ia}}(t) = y_{\mathrm{x}}^{\mathrm{Ia}} \langle \dot{M}_*(t) \rangle_{\mathrm{Ia}} = \frac{\int_0^{t-t_{\mathrm{D}}} \dot{M}_*(t') R_{\mathrm{Ia}}(t-t') dt'}{\int_{t_{\mathrm{D}}}^{\infty} R_{\mathrm{Ia}}(t') dt'} \tag{16}$$

where t_{D} is the minimum delay time for SNe Ia. `VICE` allows the user to specify any positive definite numerical value in Gyr for this parameter. It also allows the user to specify their own functional form for $R_{\mathrm{Ia}}(t)$. It then automatically normalizes the DTD in the following manner:

$$\begin{aligned} R_{\mathrm{Ia,reduced}}(t) &= \frac{R_{\mathrm{Ia}}(t)}{\int_0^{\infty} R_{\mathrm{Ia}}(t') dt'} \\ &\rightarrow \begin{cases} 0 & (0 < t < t_{\mathrm{D}}) \\ \dfrac{R_{\mathrm{Ia}}(t)}{\sum_{i=t_{\mathrm{D}}/\Delta t}^{13.8\ \mathrm{Gyr}/\Delta t} R_{\mathrm{Ia}}(t)\Delta t} & (t_{\mathrm{D}} \leq t \leq 13.8\ \mathrm{Gyr}) \\ 0 & (t \geq 13.8\ \mathrm{Gyr}) \end{cases} \end{aligned} \tag{17}$$

At the beginning of each integration, `VICE` normalizes the user-specified DTD according to equation 17. The user does not need to worry about normalizing their custom functional forms of R_{Ia}; that is done automatically. At all subsequent timesteps, the rate of enrichment from all previous stellar populations is simply the sum total from all previous timesteps:

$$\dot{M}_{\mathrm{x}}^{\mathrm{Ia}} = y_{\mathrm{x}}^{\mathrm{Ia}} \int_0^t \dot{M}_*(t') R_{\mathrm{Ia,reduced}}(t-t') dt' \tag{18a}$$

$$\rightarrow y_{\mathrm{x}}^{\mathrm{Ia}} \sum_{i=0}^{t/\Delta t} \dot{M}_*(i\Delta t) R_{\mathrm{Ia,reduced}}(t - i\Delta t)\Delta t \tag{18b}$$

The fact that $R_{\mathrm{Ia}}(t) = 0$ for $t < t_{\mathrm{D}}$ is folded into the definition of $R_{\mathrm{Ia,reduced}}$ implemented in `VICE`. Equation 18a is simply a mathematical statement that a given episode of star formation (i.e. timestep) enriches the ISM via SNe Ia some amount of time later according to the normalized rate of WD detonations at that time, and the total enrichment at a given time is simply the sum over all previous episodes of star formation.

4.3) Asymptotic Giant Branch Stars

Asymptotic giant branch (AGB) stars are evolved stars which have concluded their hydrogen and helium fuel sources. They have a core composed of carbon and oxygen with a helium-burning shell surrounding the core. AGB stars undergo dredge-up episodes in which the heavier nucleosynthetic products produced in the core are drawn to the envelope. When the star forms a planetary nebula, these products are ejected to the interstellar medium.

Naively, one would expect that a delay-time distribution similar to the treatment of SNe Ia (section 3) would suffice. However, this approach would by nature adopt the assumption that every element is enriched via AGB stars with the same delay-time distribution. This is likely true for SNe Ia because the nucleosynthesis in a white dwarf detonation should be independent of the progenitor star. Asymptotic giant branch stars have yields which are functions of mass and metallicity, which suggests that different elements would have different delay-time distributions, which would also vary with metallicity.

While this approach would not face any immediately obvious faults, it is one with hardly any theoretical or observational constraints on the relevant parameters. Instead, to retain full generality, `VICE` adopts a different implementation.

Because stars of a given mass have a given lifetime, the lookback time to an episode of star formation specifies the mass of the AGB stars associated with that population that are currently enriching the ISM. Under the assumption that stars have instantaneous post main sequence lifetimes (accurate to ~5-10%, sufficient for the single-zone approximation),

equation 6 specifies the mass of an AGB star at a given lookback time. The question that remains is thus: how many AGB stars from a given lookback time are enriching the ISM?

This is directly dependent on the star formation rate at that timestep. In addressing this question, we use a bit of mathematical slight of hand, and introduce a familiar quantity which we will refer to as the **hydrogen burning mass fraction** - the mass fraction of a single stellar population that is still on the main sequence some time following its formation. It has the following analytic form:

$$h = \frac{\int_l^{m_{\rm to}(t)} m \frac{dN}{dm} dm}{\int_l^u m \frac{dN}{dm} dm} \tag{19}$$

At first glance, it would appear that $h(t) = 1 - r(t)$. However, this is not true due to remnant masses. As we will show after further detail, the approximation $h(t) \approx 1 - r(t)$ barely fails for the single zone approximation for a Kroupa IMF.

Because $h(t)$ does not take into account remnant masses, it is necessarily $\leq 1 - r(t)$. Continuing by adopting an IMF of the general form $\beta m^{-\alpha}$ as in previous sections:

$$\begin{aligned} h &= \frac{\int_l^{m_{\rm to}(t)} \beta m^{1-\alpha} dm}{\int_l^u \beta m^{1-\alpha} dm} \\ &= \frac{\frac{1}{2-\alpha} m^{2-\alpha}\Big|_l^{m_{\rm to}}}{\frac{1}{2-\alpha} m^{2-\alpha}\Big|_l^u} \\ &= \frac{m_{\rm to}(t)^{2-\alpha} - l^{2-\alpha}}{u^{2-\alpha} - l^{2-\alpha}} \end{aligned} \tag{20}$$

The final equality is an attractive statement to make, but much more careful consideration must be taken for piece-wise IMFs like Kroupa. In that case, the second equality becomes:

$$h = \frac{\Big[\sum_i \frac{1}{2-\alpha_i} m^{2-\alpha_i}\Big]_l^{m_{\rm to}(t)}}{\Big[\sum_i \frac{1}{2-\alpha_i} m^{2-\alpha_i}\Big]_l^u} \tag{21}$$

where the summation is over the relevant piece-wise mass ranges. In the case of the Kroupa IMF, $\alpha = 0.3$ [1.3] [2.3] for stellar masses in the range $\leq 0.08 M_\odot$ [$0.08 M_\odot \leq M \leq 0.5 M_\odot$] [$\geq M_\odot$].

With the star formation history $\dot{M}_*(t)$ and the yield as a function of turnoff mass and metallicity Z, h constrains the time-derivative of the mass of a given element in the following manner:

$$\begin{aligned} \dot{M}_{\rm AGB} &= \int_0^t y(M_{\rm to}(t'), Z_{\rm ISM}(t')) \dot{M}_*(t') \dot{h}(t - t') dt \\ &\rightarrow \sum_{i=0}^{t/\Delta t} y(M_{\rm to}(i\Delta t), Z_{\rm ISM}(i\Delta t)) \dot{M}_*(t - i\Delta t)[h(i\Delta t) - h((i+1)\Delta t)] \end{aligned} \tag{22}$$

This numerical approximation may appear at first glance to have an artificial minus sign inserted into it when compared to equation 5b, but this arises simply because $\dot{h} < 0$.

In the right-hand panel of figure 1, we show numerical calculations of h against time in Gyr. At $t \approx 10$ Gyr, $h \approx 0.35$ and $r \approx 0.5$ for a Kroupa IMF. This suggests that adopting $1 - r(t)$ instead of $h(t)$ to describe the time-dependent enrichment from AGB stars from a single stellar population would systematically underpredict the enrichment of all elements produced in AGB stars. This is because it is a star's total initial mass which determines the net nucleosynthetic yield of a given element, and that includes the mass of the remnant that it will leave behind.

5) Nucleosynthetic Yields
In this section we detail the mathematical formulation of the nucleosynthetic yields implemented in `VICE`.

5.1) Core-Collapse Supernovae Yields
Enrichment from core-collapse supernovae (CCSNe) in `VICE` has an extremely simple analytic form, which arises from the assumption of instantaneous explosion (section 4.1). The form of equation 14 dictates that $y_{\rm x}^{\rm CC}$ denote the fractional of a stellar population's mass that is converted into a given element x. For this reason, it is referred to as the *IMF-integrated fractional yield*:

$$y_{\rm x}^{\rm CC}(Z) = \frac{\int_8^u m_{\rm x}(m|Z)\frac{dN}{dm}dm}{\int_l^u m\frac{dN}{dm}dm} \tag{23}$$

Under the well-founded assumption that only stars with initial masses $\geq 8M_\odot$ explode as CCSNe, this equation is simply the mathematical statement that the fractional mass yield is simply the total mass produced by each individual CCSN divided by the total mass of the stellar population.

Here $m_{\rm x}(m|Z)$ is the mass expelled into the ISM from a star with initial mass m and metallicity Z. Unfortunately, this quantity is not well understood. In practice, it is determined for individual elements via tracer particles in numerical simulations (Woosley & Weaver, 1995; Chieffi & Limongi, 2004, 2013; Limongi & Chieffi, 2018) on a grid of stellar masses and metallicities. The results are highly model-dependent, often assuming dialed-in explosion energy due to the computational expense involved in simulating supernovae. For this reason, `VICE` makes no assumptions about the user's preferred form of $y_{\rm x}^{\rm CC}(Z)$. It is left as a free parameter for the user to fully customize into an arbitrary function of metallicity Z for each individual element.

5.2) Type Ia Supernovae Yields
Enrichment via type Ia supernovae (SNe Ia), as discussed in section 4.2, is a delayed enrichment. A single stellar population's lower mass stars must first evolve off the main sequence and form white dwarves, which then explode at some rate $R_{\rm Ia}(t)$. In keeping with the formulation of *fractional* yields adopted in the treatment of CCSNe, $y_{\rm x}^{\rm Ia}$ denotes the fraction of a single stellar population's mass that is converted into an element x over the full duty cycle of the delay-time distribution. Thus the only pieces of information required are the mass of an element x produced in one instance of a SN Ia and the number of instances of SNe Ia can be expected for a given stellar population.

Maoz & Mannucci (2012) found that $N_{\rm Ia}/M_* = 2 \pm 1 \times 10^{-3}M_\odot^{-1}$, or that between 1 and 3 SNe Ia events can be expected per 1000 $M_\odot$ of star formation, with Andrews et al. (2017) and Weinberg et al. (2017) adopting $N_{\rm Ia}/M_* = 2.2 \times 10^{-3}M_\odot^{-1}$ off of their best-fit parameters. This places a theoretical upper-bound on $y_{\rm x}^{\rm Ia}$ for any given element x. In the limit that every SN Ia is a collision between two near Chandrasekhar-mass WDs, the mass available for nuclear fusion is $\sim 2.8M_\odot$. If all of this mass is converted into one element x, then $y_{\rm x}^{\rm Ia} = (2.8)(2.2\times10^{-3}) = 6.2\times10^{-3}$.

Similar to the yields from CCSNe, `VICE` allows users to customize their yields from SNe Ia, allowing any numerical value to be specified as $y_{\rm x}^{\rm Ia}$. There is little motivation for a metallicity-dependent yields from SNe Ia. It is possible that small amounts of iron-peak elements present in a WD may influence their nucleosynthetic yields; in this interest as well as for simple customizability, a future update to `VICE` will include functionality for $y_{\rm x}^{\rm Ia}$ to be a function of metallicity Z.

6) Tests
In this section we present results quantifying `VICE`'s integration time as a function of the number of elements simulated and the timestep size. As detailed in previous sections, at each timestep, `VICE` determines the enrichment of all elements from all previous timesteps. As with any other time-step style integration, the amount of data to process and thus the integration time scale with the square of the number of timesteps (i.e. $T \propto (T_{\rm end}/\Delta t)^2$).

Similarly, `VICE` treats every element independently. That is, the equations detailed in previous sections are not for any specific element - we purposefully did the analysis in full generality so that none of the simulation features in `VICE` needed to be changed to add new chemical elements. Since `VICE` conducts the same analysis for each element, we thus expect the integration time to scale linearly with the number of elements tracked per simulation (i.e. $T \propto N$).

Because `VICE` was implemented with the scientific motivation of studying the enrichment of oxygen, iron, and strontium, the first integrations were ran with these three elements, and with timesteps of $\Delta t = 1$ Myr, each simulation finished in 20.4 seconds. With these proportionalities and this calibration, we expect the following scaling relation to

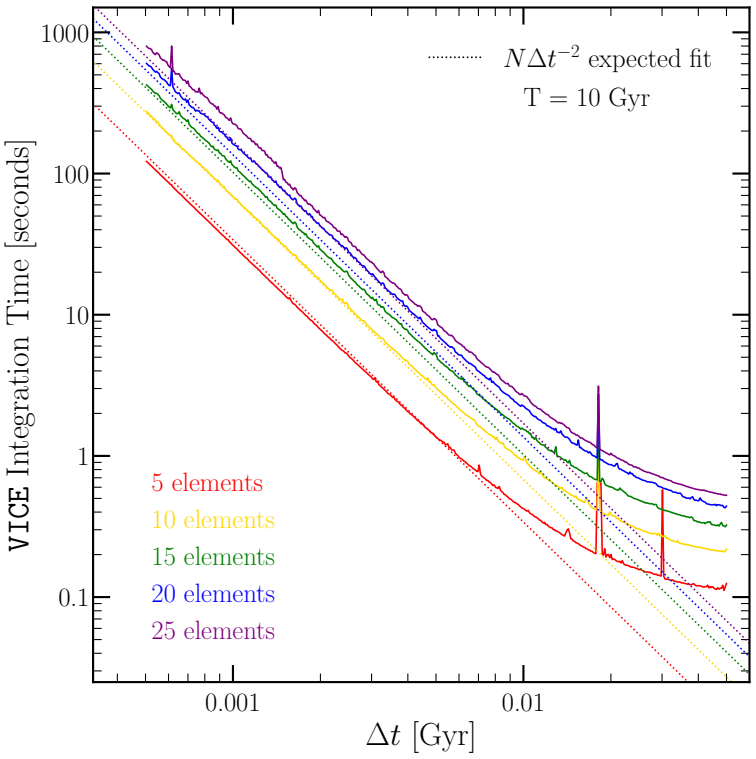

Figure 2: Timed runs with N = 5, 10, 15, 20, and 25 elements with timesteps ranging from 500 kyr to 10 Myr (solid lines) with an ending time of T = 10 Gyr. We overplot the corresponding color-coded dotted lines showing the $N\Delta t^{-2}$ expected fit. The fit does well for low N, but mildly underpredicts the integration time for higher N.

describe the time per integration in `VICE` as a function of the number of elements N, end time $T_{\rm end}$, and timestep Δt:

$$T = \left(\frac{\text{Processor Speed}}{2.7\text{ GHz}}\right)^{-1} N \left(\frac{T_{\rm end}/\Delta t}{10^4}\right)^2 (6.8\text{ seconds}) \tag{24}$$

Because 1 Myr is a relatively fine timestep, most integrations will typically not take this long. A more typical (and `VICE`'s default) timestep size would be expected to run in 68 milliseconds per element.

In figure 2 we present numerically calculated integration times for integrations over 5, 10, 15, 20, and 25 elements between Δt = 500 kyr and 10 Myr. We overplot as dotted lines in the corresponding color the expected $N\Delta t^{-2}$ fits for each line. We note first that for high N, this approximation underpredicts the integration time. Even though the mathematics is implemented uniformly for each element in `VICE`, there is still numerical overhead which increases with each element. For example, `VICE` will also take longer with more elements in determining the total metallicity at each timestep. Moreover, in writing output, `VICE` determines every [X/Y] abundance ratio - a calculation which scales with N^2. This is an effect which would be expected to mildly increase the sensitivity to the integration time for high N simulations. In practice, we find that an $N^{1.1}$ scaling performs fine for most higher N simulations.

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