Mass Spec Academy

Dos and Don’ts of typesetting in Quarto

last-modified

Here’s where you’d put some text for an abstract, if you want it. It’ll be in smaller font size than the rest of the article, though.

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Preface

The goal of this project is to create an online resource that provides comprehensive and accessible information on mass spectrometry methods used in geochronology, comprising:

- A detailed description and history of the method
- Best practices for sample preparation and analysis
- A guide to data and uncertainty analysis
- Applications, and case studies from peer-reviewed research
- Short exercises and worked solutions appropriate for graduate students.

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Part I

Overview

What is a Mass Spectrometer?

A mass spectrometer separates atoms by their atomic mass. Scientists have long known how to separate different elements based on their chemical properties. Thousands of years ago, metallic copper was first smelted from copper ore, giving rise to the Copper Age. Modern geochemical labs efficiently separate even very chemically similar elements, such as the rare earth elements, via techniques like anion exchange chromatography. These techniques separate one element from another, like separating samarium (Sm) from neodymium (Nd).

Recall that the number of protons in an atom determines the number of electrons that are needed to balance their charge. The number of electrons in an atom determines its chemical behavior —- whether and how it makes chemical bonds with other atoms. But the nucleus of an atom doesn't just contain protons, it also contains neutrons. Atoms with the same number of protons but different numbers of neutrons are called isotopes. Different isotopes of the same element behave in a chemically similar manner: you can make CO_2 with ^{12}C, ^{13}C, or ^{14}C.

The relative abundances of the isotopes of an element are key to a broad array of geological processes, including the radioactivity used as a clock in geochronology, geochemical processes that fractionate radioactive parent isotopes from their radiogenic daughter products, and temperature- and environment-dependent kinetic reaction rates. To separate isotopes by their atomic mass, we need a mass spectrometer.

Separating atoms by their atomic mass is usually accomplished by first ionizing the atoms, for instance by stripping an electron off to create an ion with a +1 positive charge. The ions can then be separated according to their mass-to-charge ratio, often denoted m/z, using electric and magnetic fields.

Background Contents

1 Template Chapter

⚠ Warning

This Mass Spec Academy content is under construction.

1.1 Basics

Write using Markdown syntax, and find a quick tutorial here: My link text.

Check out template_chapter.qmd on VS Code to see how this is all typeset.

To be consistent across the project, let's typeset the mass number of an isotope with a LaTeX superscript, like ^{12}C. The element symbol's letters go outside the dollar signs. Likewise for a chemical formula, like CO$_2$. Numbers and uncertainties are in unicode, like 10 ± 2 Ma, rather than LaTeX like 10 ± 2 Ma.

1.2 This is a top-level section, like Headings and Labels

After the title of the section, you can optionally add a label in curly braces {} so that you can refer to it later. The `#sec-` at the start of the section label is mandatory for Quarto. Quarto will yell at you if you have accidentally duplicated a label name from another chapter so that you can change yours.

To refer to this section anywhere in the book, just write `@sec-template-headings`.

With a labelled section like this one, you can link back to Section 1.2. If you want to just refer to the section number (without the word "Section"), then use `[-@sec-template-headings]`. Please use hyphens instead of underscores in your label names to keep LaTeX happy.

Relevant headers and references docs

1.2.1 This is a subsection, like Ion Counter Types

1.2.1.1 This is a subsubsection like Dynode Voltage Schemes

1.3 Figures

The Quarto syntax for a figure looks like

```
![Caption text here](relative_path_to_figure.png){#fig-my-label fig-alt="Alt text" width="XX
```

Here's an example. Use a blank line between the text and the figure syntax so that it isn't set inline. Figures are numbered sequentially and can refer to them if you add a label, just like for sections. The label must start with `#fig-` and don't use underscores please. Also, if the contents of the curly braces appear below the figures instead of styling the figure, it's because you used commas between the options that appear inside the curly braces (don't do that).

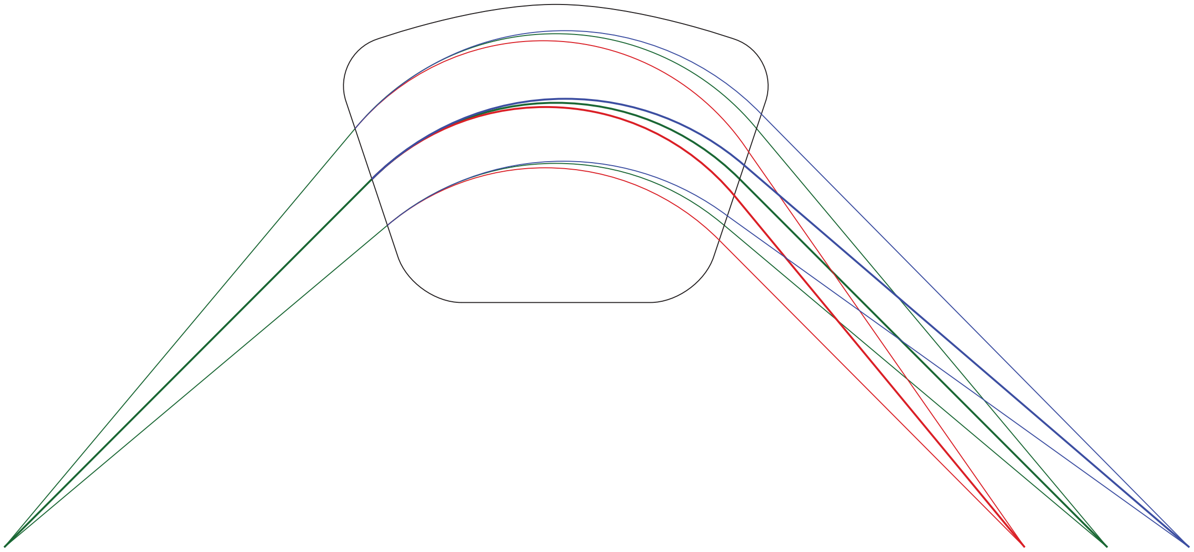


Figure 1.1: An extended geometry magnetic sector mass spectrometer.

Relevant Quarto Docs for many more figure options

Another way to format a figure

1.4 Citations

Export your references from your reference manager or from the online journal article in a BibTeX format, then add the work to the `references.bib` file. The name of the bibliography entry is the first element after the opening curly brace. You can reference the entry in the text using an `@` followed by the name of the entry. For instance, Wang et al. (2021) typesets a reference to an atomic mass table reference.

All the usual inline reference formats are included, like (Wang et al. 2021) or (e.g., Wang et al. 2021) or (Wang et al. 2021; Yergey and Yergey 1997).

Your cited reference will automatically be added to the References section.

Relevant citations docs

1.5 Equations

You can typeset inline equations like $F = ma$ and display-style equations like:

$$\sigma_z^2 = \sigma_x^2 \left(\frac{\partial z}{\partial x}\right)^2 + 2\sigma_{xy}^2 \left(\frac{\partial z}{\partial x}\right)\left(\frac{\partial z}{\partial y}\right) + \sigma_y^2 \left(\frac{\partial z}{\partial y}\right)^2 \tag{1.1}$$

Typeset equations like Equation 1.1 using LaTeX syntax. VS Code with the Quarto extension gives you a nice interactive preview of the display-style equation on the left-hand panel if you hit the “Preview” button above the first double dollar sign. A display equation will be numbered if you include a label after the final double dollar sign, like `{#eq-unct-propagation-xyz}` above.

For more complicated equation environments, you’re best off with a trial and error approach, but Quarto seems to include many of the usual (e.g., amsmath) packages by default.

Relevant equations docs

1.6 Callout Blocks

> **Note**
>
> We could use callout blocks in the html version of our book. This might be helpful for text asides in a less formal tone.

> **What are the three parts of a mass spectrometer?**
>
> Perhaps we could use collapse callouts for the end-of-chapter questions and answers?

Relevant callouts docs

1.7 Code

Check out background.qmd for a short Python code that creates a figure output. The code that created that figure is automatically included on the website as a collapsible code block above the figure. You can edit and execute the Python inside VS Code and then preview in Quarto to see the results.

If you wish to add an executable code block, then make sure to un-comment the `jupyter: python3` line from the header at the top of the document by removing the `#` in front of it.

Relevant code block docs

2 Physics and Chemistry Background

2.1 Forget the Spectrometer, What is a Mass?

2.1.1 SI units for mass

The SI unit for mass is the kilogram, but samples analyzed for mass spectrometry are usually much smaller. The table below lists some typical sample sizes for geochemistry, both as SI terms with prefixes and as fractions of a gram. As we will soon learn, the number of atoms in a gram depends on the atomic mass of the atoms. The third column gives the number of atoms of that mass. It starts with atoms of mass 12 unified mass units (i.e., ^{12}C), but you can hover your slider over the blue atomic mass and drag left or right to increase or decrease its value.

Table 2.1: SI prefixes for small things.

Mass with Prefix	Mass in grams	Atoms of ^{12}C	Atoms of ^{238}U
kilogram	10^3 grams	6×10^{26}	3×10^{25}
gram	1 gram	6×10^{23}	3×10^{22}
miligram	10^{-3} grams	6×10^{20}	3×10^{19}
microgram	10^{-6} grams	6×10^{17}	3×10^{16}
nanogram	10^{-9} grams	6×10^{14}	3×10^{13}
picogram	10^{-12} grams	6×10^{11}	3×10^{10}
femtogram	10^{-15} grams	6×10^{8}	3×10^{7}
attogram	10^{-18} grams	602214	30357

2.1.2 Other units for mass

The familiar (and perhaps unfamiliar!) SI prefixes down to the attogram still don't reach a small enough value to easily compare the masses of single atoms, like ^{238}U and ^{235}U. For that, we'll need a new unit, the unified mass unit, also known as the Dalton (symbols: u or Da). The unified atomic mass unit is not in the SI, but it's commonly used in physics and chemistry for very small masses, like the mass of a single atom or molecule. It's defined as $\frac{1}{12}$ the mass of a ^{12}C atom. That's about 1.660539×10^{-27} kilograms. The equivalent unit Dalton is more widely used in the organic chemistry community.

What about the atomic mass unit, or amu? This very similar unit was used widely in the mid-twentieth century but was defined differently by physicists and chemists. It was formally abandoned in 1961, replaced by the unified atomic mass unit and the Dalton, and assigned unique unit abbreviations. However, many scientific communities still use amu to abbreviate the unified atomic mass unit. The inorganic mass spectrometry community is among them, and this textbook will use amu below.

2.1.3 Atomic masses of your favorite isotopes

The isotope ^{12}C is the only isotope with an integer mass (it has a mass of 12 amu). Other isotopes have non-integer masses, which are determined to high precision by nuclear physicists. Masses and 1σ uncertainty in parentheses are from Wang et al. (2021):

- ^{1}H has a mass of 1.007825031898(14) amu
- ^{86}Sr has a mass of 85.9092607309(91) amu
- ^{144}Nd has a mass of 143.9100873(25) amu
- ^{208}Pb has a mass of 207.9766521(13) amu
- ^{238}U has a mass of 238.0507882(20) amu

Isotopic masses aren't integers for several reasons. First, neutrons and protons don't have exactly the same mass. Neutrons are slightly heavier than protons (1.0087 vs. 1.0073 amu, respectively). But an atomic mass is different from the sum of the masses of its protons, neutrons, and much lighter electrons. The difference is the binding energy of the atom and specifically the nucleus, or the energy released by the formation of the nucleus from its constituent parts. This energy of fusion, which powers the sun and stars, can be converted to mass via Einstein's famous equation $e = mc^2$. So the combined mass of 6 protons + 6 neutrons + 6 electrons is 12.0989 amu, and the difference between that mass and the 12 amu mass of a ^{12}C atom is the energy released by putting the atom together.

The chemical energy released by forming a molecule out of atoms is small relative to the nuclear forces responsible for forming atoms, so the molecular mass of a molecule is very close to the sum of the atomic masses of its atoms. Note that two molecules with the same chemical formula might have two different molecular masses. For instance, $^{12}C^{16}O_2$ will have a different molecular mass than $^{13}C^{16}O_2$ will have a different mass than $^{12}C^{18}O^{16}O$. These three molecules, all with a different molecular mass, are called isotopologues.

Because each isotope has a slightly different mass, different atoms and/or molecules may have very similar masses. For instance, the mass of ^{40}Ar is 39.96238 amu, the mass of ^{40}Ca is 39.96259 amu, and the mass of ^{40}K is 39.96400 amu. Their proximity in mass makes these isotopes difficult (but not impossible) to separate with mass spectrometers. The more atoms a molecule has, the more opportunities isotopic substitution has to create near-overlaps. For instance, natural U is often measured by TIMS as UO_2^+ after adding a tracer containing synthetic U isotopes.

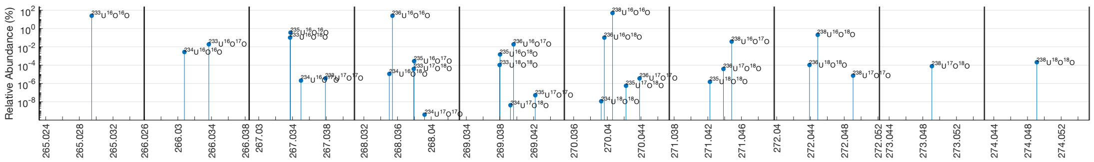


Figure 2.1: Uranium oxide (UO_2) isotopologues for a natural U sample with a ^{233}U-^{236}U tracer added. The ^{238}U/^{236}U ratio is 0.5 for this sample, and the tracer ^{233}U/^{236}U is 1. Click to enlarge the figure.

2.2 Energy, Electricity, and Magnetism

To separate dissimilar objects like minerals or legos, one good strategy is to place them all together and then sort through and choose different elements from the pile. A chemical reaction might dissolve or precipitate one element and leave another behind. However, isotopes of the same element have nearly identical chemical behavior. Mass spectrometers don't inspect and sort a stack of static individual atoms like sorting legos, and they can't rely on chemical reactions to sort isotopes.

Instead, mass spectrometers move the atoms by first ionizing them and then manipulating the ions with electrical and magnetic forces. The resulting kinetic changes in the isotopes' motion depend on their atomic or molecular mass, which can be exploited to separate different isotopes. Once separated, the streams of ions in motion must be measured by sensitive electronic instruments. Here again, the ions' electrical properties are important.

2.2.1 Energy

$$KE = qV = \frac{1}{2}mv^2 \tag{2.1}$$

```python
import numpy as np
import matplotlib.pyplot as plt

kg_per_amu = 1.66e-27
mass_amu = 238
mass_kg = mass_amu * kg_per_amu
velocity_meters_per_second = np.linspace(0, 2, 100)
kinetic_energy_joule = mass_kg * velocity_meters_per_second ** 2

fig, ax = plt.subplots()

ax.plot(velocity_meters_per_second, kinetic_energy_joule)
```

```
ax.set_xlabel('Veclocity (m/s)')
ax.set_ylabel('Kinetic Energy (J)')
ax.set_title('Quadratic Function')
fig.tight_layout

plt.show()
```

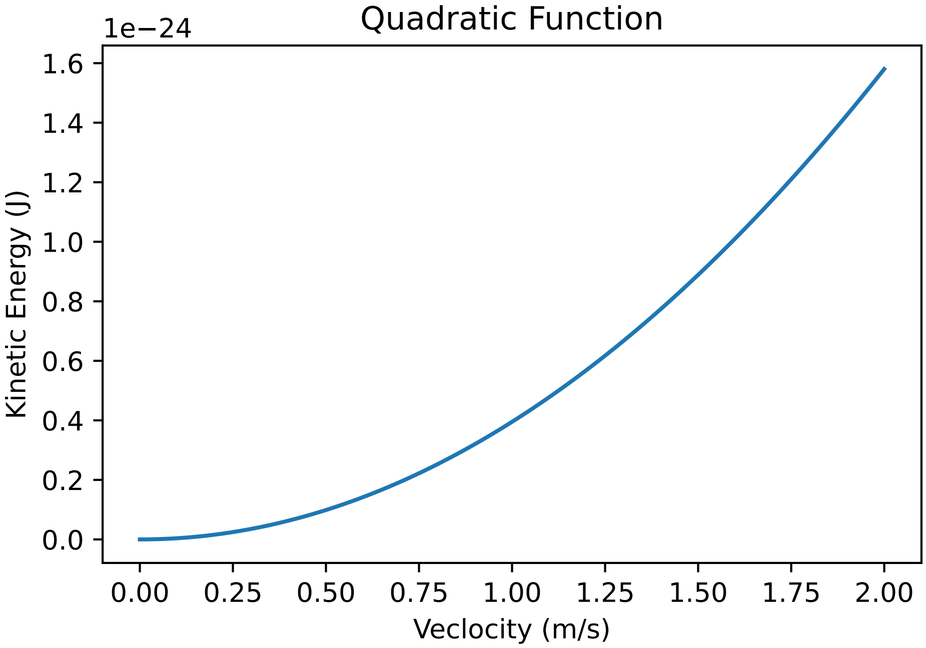
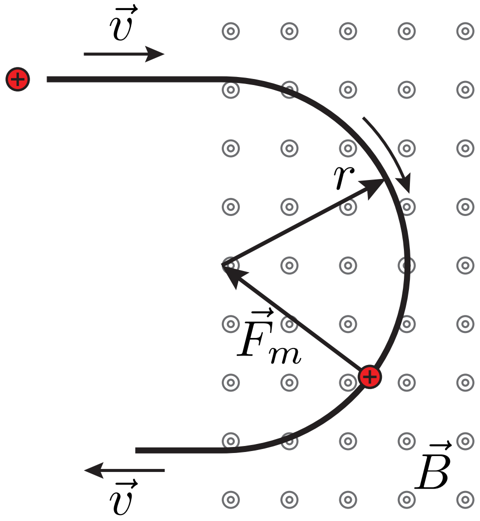


Figure 2.2: Kinetic energy as a function of velocity for ^{238}U



Magnetic force acts on a positively charged ion. Figure after Bill O.

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3 Ion Sources

Figure 3.1: One of the beta unit calutron sources. ORNL Photo 24574, from Yergey and Yergey (1997).

Part II

Contributors

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Stephen Cox is an isotope geochemist who measures noble gases to date rocks and minerals. His interests extend from deep time thermochronology in the western United States to the geology of winemaking. He has a PhD from Caltech and has been at Lamont-Doherty Earth Observatory since 2017.

Stephen Cox Geology

Noah McLean

My research interests center around using high-precision isotopic measurements to study geologic and geochemical systems, with a focus on U-Pb geochronology. I often develop new statistical methods to better understand and interpret data, and I frequently work with other scientists to integrate these approaches into scientific workflows.

Cemil Arkula

Empty

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profile/IMG_6742.mov

Max K. Lloyd

Max Lloyd is a stable isotope geochemist and Assistant Professor at Penn State. Max and his lab pull small bits off of large organic molecules, and put them into gas-source mass spectrometers to analyze their clumped and position-specific isotope compositions.

Max got his PhD in Geochemistry from Caltech in 2017. He spent two years as an Agouron Geobiology Postdoctoral Scholar at UC Berkeley working with Daniel Stolper. He started at Penn State in 2020.

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Hi there! I'm Fatema Panahi

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Keywords:

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- mass spectrometry
- instrumentation
- isotope geochemistry
- stable isotopes
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Marissa Tremblay is an Assistant Professsor at Purdue University in the Department of Earth, Atmospheric, and Planetary Sciences. Marissa is the PI of the Thermochronology @ Purdue (T@P) research group, which includes a noble gas mass spectrometry facility focused on measurements of comsmogenic and radiogenic noble gases.

Part III

Mass Spectrometry Overview

4 Mass spec history

4.1 1890s-1920s: Early developments

4.1.1 Cathode ray tubes

In the 1890's scientists worked to understand atomic structure. This exploration eventually lead to the discovery of cathode rays specifically to determine mass, which we now call electrons. In probing cathode rays he deflected them magnetically or electrically, and then compared the heat generated when they hit a thermal junction. The deflection allowed him to calculate mass and the heat generation allowed him to calculate energy. By discovering these subatomic electrically charged particles he won the nobel prize for this in 1906

JJ Thomson continued this work with his research assistant FW Aston. They would deflect accelerated gases using a magnetic and electric field and measure that deflection using a photographic plate in the path of the ion beam (Figure 4.1). The physical dispersion was measured and due to the presence of two dispersion paths the two stable isotopes of neon were discovered in 1912, the first time stable isotopes were measured. The glass apparatus that the subatomic particles were accelerated through is a cathode ray tube, and is a predecessor to the modern day mass spectrometer. Aston continued the work combining magnetic and electronic separation increasing the mass resolving power of the instruments .

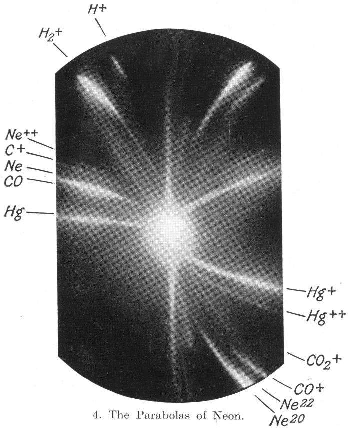


Figure 4.1: Deflection of different isotopes of neon by JJ Thomson and FW Aston captured on photographic film

4.1.2 Electron impact sources

Alternatively, in 1917 AJ Dempster published a work on positive rays largely considered to be the first description of an electron ionization source (Dempster 1918). He directed a positively charged beam at a solid surface generating ions he could determine a mass to charge ratio. He continued this work and eventually determined the stable isotopes of lithium and magnesium using this technique. Furthering the techniques developed by Dempster, W Bleakly was able to generate a monoenergetic beam of electrons to ionize gases in 1929 (Bleakney 1929). The beam in this type of instrument traversed a 180 ° magnetic field and was deflected in a circle to the detector.

4.2 1930s: The first mass spectrometers

Due to the size and complexity of the 180 ° magnetic field early spectrometers, they were difficult to build and maintain making them a relatively rare tool. In 1940 A Nier developed a mass spectrometer in which the ion source and the detectors were removed from the influence of the 60 ° magnet. These sector field mass spectrometers greatly reduced the power consumption of the instruments, decreased complexity, and did not decrease the mass resolving power. With the knowledge that was gained during the war expansion, he published his seminal paper in 1947, describing the basis of most mass spectrometers that are still used today (Nier 1947). The Nier-Johnson or double focusing mass spectrometer combined the sector magnet with an energy filter allowing for pure separation by mass, a design that is still the norm for high mass resolution instruments.

4.3 1940s-1950s: The Manhattan Project and World War II

World War II greatly accelerated the pace of scientific development in physics and chemistry as world powers competed to develop new weapons, production techniques, and energy sources. While international collaboration and public dissemination of research ground to a halt during the war years, scientists continued working in secret on much of the same basic research—alongside a focus on applications to wartime policy goals, particularly nuclear weapons development. During the war, massive industrial operations like the Manhattan Project focused on isotope separation technology and the physics of nuclear decay and chain reactions. After the war, many of the scientists who worked on these projects returned to basic research, publishing a wave of new publications based on previously secret wartime research. These developments in the late 1940s and 1950s laid the groundwork for the modern field of isotope geochemistry by bringing the tools of nuclear war to bear on chronology and chemical processes in the geosciences.

4.3.1 The Manhattan Project

Nuclear weapons require a sufficient mass of concentrated fissile material (known as a *critical mass*) to maintain a nuclear chain reaction. Obtaining a critical mass involves mining and chemical separation of uranium and subsequent isotope enrichment to obtain an enrichment of at least 5.4% uranium-235ref (usually much higher), which is the level required to sustain a chain reaction. The critical mass depends on the activity of the fissile species and its concentration or grade. For example, the critical mass of a sphere of metallic uranium-235 is around 50 kg, whereas for plutonium-239 it is only around 10kg ref. At 20% enrichment of uranium-235, the critical mass is well over 500 kg ref.

In addition to understanding the parameters of criticality and sourcing raw materials, the success of the Manhattan Project depended on achieving sufficient enrichment of fissile species. Natural uranium is about 0.7% uranium-235, and while enriching it to just over 5% provides the theoretical possibility of criticality, weapons charges with masses in excess of a ton are impractical. A standard definition of "highly-enriched uranium" is over 20% uranium-235 ref, but in practice weapons-grade uranium is usually over 90% uranium-235.

Uranium isotope enrichment can be performed in multiple ways, and most modern enrichment facilities use gaseous diffusion of UF_6 in a chain of gas centrifuges to gradually separate the heavier and lighter natural isotopes of uranium ref. However, the first uranium bomb produced during the Manhattan Project (the "Little Boy" gun bomb) used uranium produced by the Calutrons in the Y-12 enrichment facility at Oak Ridge ref. The Calutrons, so named because they were developed by Ernest Lawrence at The University of California and used large magnets originally built for cyclotrons, were essentially enormous mass spectrometers in which UCl_4 was ionized by hot filaments and then separated by travel through a magnetic field, the same way a mass spectrometer mass analyzer separates isotopes. However, rather than measuring nA and smaller ion beams using sensitive electronics, the Calutrons collected grams of enriched uranium from ion beams in the tens of mA in graphite collector cups that were later burned to allow recovery of the uranium metal ref.

4.3.2 Postwar science

After the conclusion of the war, the physicists and chemists who had worked on the chemistry of isotope enrichment and the physics of nuclear weapons returned to other realms of basic and applied science. The same physics understanding that allowed scientists and engineers to construct nuclear weapons contributed to an understanding of the decay of radioactive nuclides to produce enrichments in radiogenic daughter products in natural materials, which is the basis for radiogenic isotope geochemistry. The principles underlying the chemical separation of isotopes, whether through electromagnetic separation or gaseous diffusion, applied as well to the separation of isotopes through natural geochemical processes, which is the basis for stable isotope geochemistry.

4.3.2.1 Technological developments

In addition to the boosts that the underlying science of geochemistry received from the Manhattan Project, the early mass spectrometers pioneered by AO Nier and others benefited directly from the work on Calutrons and other scientific and industrial instruments during the war years. Rapid advances in vacuum systems and instrument design occured in this era. John Reynolds introduced the static vacuum noble gas mass spectrometer in 1956, dramatically improving the sensitivity of these instruments and paving the way for realistic measurement of noble gas samples from rocks and minerals ref. This in turn enabled the rapid growth of the K/Ar dating technique, which allowed geochemists to produce a quantitative Geologic Time Scale and which dominated the next several decades of geochronology before being largely displaced by the related ^{40}Ar/^{39}Ar technique and U/Pb geochronology.

4.4 1960s-1970s: Diversification of techniques

4.5 1980s-1990s: Commercializaiton and plasma sources

Houk et al. (1980) and Date and Gray (1981) developed inductively coupled plasma mass spectrometry (ICP-MS). Gray (1985) coupled ICP-MS with laser ablation (LA) systems (as a sample introduction). Soon after their development ICP-MS (in 1983) and ICP-MS coupled with LA (1990) became comercially avaialble and experienced great improvements, which made them one of the most dominant techniques for trace, ultratrace and isotope analysis.

The development of matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS) and electrospray ionization mass spectrometry (ESI-MS) Tanaka et al. (1988) enabled soft ionization large biomolecules. Earliest succesful analyzes on biomolecular on macromolecules using soft ionization published in late 1980's (Fenn et al. 1989, 1990). Fenn and Tanaka (together with Wüthrich) received the Nobel Prize for chemistry in 2002 ((**https://www.nobelprize.org/prizes/chemistry/2002/popular-information?**)/.). Nowadays, MALDI and ESI are soft ionization techniques that are combined with various mass analyzers to analyze proteins, peptides, syntheic polymers, small oligonucleotides, carbohydrates andlipids

THe rapid improvements and development were triggered by extensive application fields, which included investigation of the hazardeous waste disposal (approved by US Enviremental Protection Agency), space explorations ((**https://science.nasa.gov/mission/galileo-jupiter-atmospheric-probe?**)/)

:

4.6 2000s-modern: Multicollection and modern electronics {#sec-hist-2000s+}

4.7 Further Reading

(Griffiths 2008) (De Laeter and Kurz 2006)

5 Mass Spectrometer Components

General outline of a mass spectrometer

Diagram with parts labeled. Ion optics will point to several different pieces.

5.1 Sample introduction systems

Sample introduction systems can be organized by the physical form (phase) of the material it handles. Fundamentally different strategies are needed depending on whether the sample is a solid, liquid, or gas. The right introduction system for your specific application could also depend on your analytical goal. For example, you might need to add a tracer to help you quantify amounts of certain analytes, or use exploit chemical or physical processes to remove a problematic contaminant. Here, we'll organize introduction systems by sample phase.

5.1.1 What makes a good sample introduction system?

Regardless of the physical form of the sample, all sample introduction systems adhere to (or strive for) a few guiding principles: 1. Vacuum: Slow enough introduction rate that the instrument remains at vacuum 2. Stable: Introduction of material (and thus ion beams) are stable over time or change only gradually, ideally in a manner that does not fractionate the sample (or if it does fractionate, does so reproducibly) 3. Identical treatment: System strives to treat samples and standards identically, and switch between samples and standards easily without changing the state of the instrument.

5.1.1.1 The vacuum constraint

Mass spectrometers require high or ultra-high vacuum to operate. If the ions that we've worked so hard to separate from each other hit other particles in the instrument, they'll get knocked off course, lose energy, and show up in the wrong place. The technical term for this is the **mean free path**, which chiefly depends on pressure and quantifies how long the average particle can travel in a straight line before hitting another particle. See XXX for more details on the mean free path and how to calculate it. So, when working correctly, a mass spectrometer needs a low pressure and (thus) a long mean free path.

However, analyzing a sample, by definition, adds stuff to the instrument and makes the vacuum worse. So, the way that and rate at which we can introduce a sample to the instrument is constrained by how many particles we can tolerate (before the mean free path is too short) and the rate and which the instrument can remove them. Larger samples create brighter ion beams, more counts, and thus higher precision. But the size of samples are fundamentally limited by how much added material a mass spectrometer can handle. Every sample introduction system is bounded by this constraint and must design around it.

For example, suppose we need a mean free path of at least 100 m, so that nearly all ions avoid collisions along the ~1 m flight path of our mass analyzer and our mass resolving power doesn't degrade. At room temperature, this requires a pressure no higher than about 10^{-9} bar for molecules the size of the main components of air. If vacuum is maintained using a turbomolecular pump with a pumping speed of 100 L/s (which is pretty standard), from $Q = SP$, we can add sample at a rate no higher than $100\ \mathrm{L/S} \times 10^{-9}$ bar $= 10^{-7}$L bar/s. For an ideal gas at room temperature, this corresponds to $\frac{PV}{RT} = 10^{-7}/0.083/298 \approx 4 \times 10^{-9}$ moles/s, or about 0.25 μmoles per minute. This constraint may be easily met in systems working on small amounts of material, but it still governs the design of the sample introduction system

Beyond this fundamental constraint, two additional constraints related to vacuum that influence the design of sample introduction systems are: 1) if they were handled by humans, most samples are (or at some point were) at atmospheric pressure; and 2) many ion sources require (or operate more efficiently in) environments where the mean free path is much shorter than 100 m. Getting samples from atmospheric pressure to whatever pressure the ion source requires (anywhere from $< 10^{-8}$ to > 1 bar depending on the instrument), and then from the pressure in the ion source to the (often) lower pressures required by the mass analyzer at the slow rates required by the $Q = SP$ constraint above is a throughline that controls how mass spectrometers are designed. How different inlet systems solve these constraints depends on the phase in which the material is analyzed.

5.1.1.2 Stability constraint

5.1.1.3 Identical treatment

5.1.2 Gases

Adding gases to a mass spectrometer is, in principle, easy because gases will act to equalize pressures across the space provided them. So, if the pressure in our ion source is lower than in the sample reservoir, gas will flow into our instrument at a rate that we can control based on the conductance at the interface. In practice,

5.1.2.1 Viscous leak (e.g., Dual-inlet)

5.1.2.2 Capillary leak (e.g., Continuous-flow)

5.1.3 Liquids

5.1.3.1 Wet plasma

5.1.3.2 Desolvating nebulizer

5.1.3.3 Liquid chromatograph

5.1.4 Solids

5.1.4.1 Laser ablation

5.1.4.2 Ion bonbardment (SIMS?)

5.1.5 Other

Clean lab (a bunch of chemistry)

Noble gas extraction line

5.2 Ion sources

5.2.1 Electron Impact

5.2.2 Thermal ionization

5.2.3 Inductively Coupled Plasma

5.2.4 Secondary ion sources

5.2.5 Other ion sources

Glow discharge Electrospray MALDI Laser desorption RIMS

5.3 Analyzers

5.3.1 Magnetic sectors

5.3.2 Electrostatic analyzers

5.3.3 Quadrupoles

Quadrupole mass analyzers generate electric fields through which only ions of certain mass to charge ratios are able to pass. As shown in the figure -need fig-, ions enter the quadrupole along it's z-axis. Those with m/z within the selected range will maintain a stable trajectory along the z-axis and reach the spectrometer's detector. The electric fields will destabilize the paths of ions with m/z outside the selected range, knocking them "off course" and preventing them from passing through the analyzer.

Dynamic.

Analyzer vs. filter? filtering vs. bending?

How does quadrupole mass filtering work?

Quadrupole mass analyzers use four parallel rods that are connected in cross-wise pairs. A potential of (U+Vcos t) is applied to one pair, while a potential of -(U+ t) applied to the second pair. Here, Vcos t represents an alternating RF voltage and U represents a DC voltage ("DC offset"). The applied potentials create orthogonal electrical fields–one in the x-plane, and one in the y-plane–that interact differently with ions of different m/z.

In the X-direction, low m/z ions generally follow the RF component of the field, gain energy, and oscillate with increasing amplitude until they collide with the rods. This creates a "high-pass" filter in the X-direction that allows only heavier ions to maintain their trajectory.

In the Y-direction, the DC component of the field has a "de-focusing" or destabilizing effect, but the RF component can keep lighter ions on course by periodically correcting their paths. In this direction, the applied electric fields create a "low-pass" filter through which only lighter ions can maintain their trajectory. By manipulating the RF and DC components of the field, the high and low-pass filters can be set to resolve individual atomic masses.

Some math! or **More details!** or **How are potentials calculated?**
- follow an ex: stability of ion of a single mass - mathieu equation and "stability triangle"

Advantages of quadrupoles

5.3.4 Collision/Reaction cells (CRCs)

The purpose of a collision/reaction cell (CRC) is to use an added gas within the cell to mitigate spectral interferences, either via collision of interferents with gas molecules or reaction of interferents or interferred ions . CRCs are most typically used in conjuction with ICP-source instruments, and are placed before the mass analyzer to filter ions or interferences of interest.

A CRC is typically housed within an RF multipole (either quadrupole, hexapole, or octopole), which serves to focus the ion beam. Some CRCs also induce an axial electrical field (along the length of the cell) in order to slow ions down or speed them up, depending on the type of reaction. The two primary CRC modes are collision mode and reaction mode.

In collision mode, an inert gas such as He or H_2 is used to collide interferents. One general guiding principle of collisions is that the cross-sectional area of polyatomic ions is generally larger than the analyte of interest. This results in more collisions of polyatomics than single ions with the reaction gas.

> CID (Collision Induced Dissociation) - Generally, polyatomic ions produced in the plasma collide with neutral gas molucules in the collision cell, resulting in dissociation of the polyatomics.
>
> KED (Kinetic Energy Descrimination) - Collisions occur between an ion and the collision cell gas. These collisions result in the transfer of kinetic energy from the ion (high kinetic energy) to the gas molecule (very low kinetic energy). By the time the ion exits the cell, it has considerably reduced kinetic energy and is easily filtered out by a kinetic energy barrier after the cell. See Yamada 2015 for an extended explanation of KED processes.

In reaction mode, a gas is used to react with either the primary ion of interest or the interferent in order to mitigate the interference.

> Charge transfer reactions: A charge transfer reaction results in the transfer of the charge from one ion or molecule to another

Example

Ammonia (NH_3) gas can be used to neutralize Hg^+ to Hg^0, thereby removing the Hg interference on Pb. This is a two step reaction that first neutralizes Hg^+ by transferring the charge to form NH_3^+; NH_3^+ then reacts with NH_3 to form NH_2 and NH_4^+:

$$Hg^+ + NH_3 = Hg^0 + NH_3^+$$

$$NH_3^+ + NH_3 = NH_2 + NH_4^+$$

Atom transfer (mass shift): Atom transfer or mass shift reactions involve the creation of new molecules, effectively mass shifting an ion of interest to a new mass.

ℹ Example

Polyatomic interference of ^{87}Sr on ^{87}Rb prevents their separation using traditional mass analyzer techniques. Within a reaction cell, the user can add SF_6 gas to react $^{87}Sr^+$ to $^{106}SrF^+$. Rb is non-reactive with SF_6. Rb is now measured on-mass as ^{87}Rb, whereas Sr is now measured mass-shifted as $^{106}SrF^+$.

The likelihood of a reaction occurring depends upon the thermodynamics of the reaction, which is different for every element and gas. Some helpful resources for understanding reaction gas kinetics can be found below:

Link to element reactivities for the periodic table from the research group of Dr. Diethard K. Bohme at the University of York.

Link to Agilent reaction data table based on sensitivity data for no gas, O_2, NH_3, and H_2.

5.3.5 AMS

5.3.6 Time of Flight

5.3.7 Orbitrap

5.3.8 Others

FT-ion cyclotron resonance

5.3.8.1 Amplifiers

Capacitive

Resistance-based

5.4 Detectors

There are several different types of detectors integrated into mass spectrometers. Three general capabilities of the ideal ion detector include: (1) acceptance of ions, (2) 100% efficiency, or no signal loss, and (3) no bias between detectors during simultaneous collection of multiple ion beams.

Various types of detectors are described below:

5.4.1 Faraday detector

5.4.2 Electron Multipliers and/or Ion Counters

Ion counting and the use of electron multipliers have been incorporated into mass spectrometry to detect and measure every ion of low-intensity ion beams, typically less than 10ˆ6 counts per second (CPS). The physical process that allows electron multipliers, or ion counters, to operate is secondary ion emission. The general principle of secondary electron emission is a particle, or ion, impacts a high-voltage surface, or dynode, causing the release of secondary electrons from the outer layers of atoms. The number of electrons produced by an impact is dependant on the type of particle hitting the surface (i.e. positive ion, negative ion, electron, etc.), the angle of contact between the particle and the surface, the mass and energy of the incoming particles and the condition of the surface. The electrons produced by this initial collision are directed down the detector by an electric potential gradient, generating even more secondary electrons each time a collision occurs between an electron and the dynode surface inside the detector until they reach an output device at the end of an ion counter, where a resultant pulse is produced that is electronically processed. Continuous-dynode electron multipliers, discrete-dynode electron multipliers, and Daly detectors are three types of ion counters used for the detection of low-intensity ion beams discussed below.

5.4.2.1 Secondary Electron Multipliers

Discrete dynode electron multipliers are detectors that amplify electron signals through a series of individual electrodes called dynodes. When a primary electron strikes the first dynode, it releases multiple secondary electrons, which are accelerated to the next dynode by an applied voltage. This process repeats across several dynodes, resulting in exponential signal amplification. Discrete dynode designs offer high gain, fast response times, and are widely used due to their sensitivity and reliability.

5.4.2.2 Channeltrons

Continuous dynode electron multipliers are curved lead-silicate glass tubes that have the ability to detect both positive and negative ions, electrons and photons. A potential between 2200 and 3200 V is applied to the top, or input end, of a continuous-dynode electron multiplier and decreases steadily to ground state at the output end of the detector. Secondary electrons generated at the input end of the detector are driven down the channel to a collector by the potential gradient generating even more secondary electrons each time the particles some in contact with the inner surface walls of the detector.

5.4.2.3 Daly Detectors

Daly detectors are specialized ion detectors designed to reduce noise and extend detector life. In this system, ions strike a metal electrode (often called a conversion dynode), releasing secondary electrons. These electrons are then accelerated toward a scintillator, where they generate photons. The resulting photons are detected by a photomultiplier tube (PMT), which produces the final output signal. This indirect detection method minimizes direct ion contact with sensitive components, enhancing longevity and reducing background noise.

5.4.3 Other

AMS Detectors (ion counters with information on energy). Gas ionization detectors.

Array detectors

5.5 Ion optics

5.5.1 Ion lenses/deflectors

5.5.2 Using magnets as ion optics

5.5.3 Retardation lenses

5.5.4 Zoom/dispersion lenses

5.6 Vacuum Systems

A large amount of the design and mechanical components of mass spectometers are dedicated to production and maintenance of regions with a very low density of gas - typically several order of magnitude lower gas concentration than atmosphere. The term “vacuum” is typically applied to gas pressures significantly below atmospheric. A “high vacuum” is “low pressure”. The SI unit for pressure is the pascal, with the symbol Pa and in SI base units are kg/m/s^2, although workers commonly continue to use non-SI units such as bar (or even more commonly, mbar) and torr, where 1 mbar = 0.750062 torr = 1 hPa. Conveniently, pressures are typically reported in orders of magnitude, so for the purposes of vacuum systems in mass spectrometers, mbar ~ torr ~ hPa.

High vacuums are useful for several reasons, the importance of each depends on the type of mass spectrometer and analysis. When an ion beam moves through space, uncontrolled ion-gas interactions are typically deleterious because they induce ion scattering and energy loss. The mean-free-path of an ion - the average distance over which an ion cna travel without colliding with a gas particle - is a useful concept. At atmospheric pressure, the mean free path is only 10s of nanometers, whereas under pressures more typical of mass spectrometers, ca 10^-7 to 10^-10 hPa are 10s to 100s of kilometers, much longer than the typical drift length of ion beams in mass spectrometers.

Ions are often accelerated using high-voltage components. Unfortunately, residual gas between two electrodes at differing electrical potential can cause arcing and high voltage discharge. This can damage sensitive components, disrupt measurements, and pose safety hazards. The breakdown distance in dry air, for example, for a potential difference of 8 kV, is ~5 cm. In contrast, at a pressure of only 10^-2 hPa, the breakdown distance decreases to 1 m, permitting components at different potential differences to be closely spaced.

For mass spectrometer measurements of gasses, the vacuum quality can also contribute to sample contamination. For example, Ar is 0.94% of dry air, so for geochronology measurements of radiogenic ^{40}Ar, the higher the vacuum, the better the sample-to-blank ratio.

5.6.1 Gas flow at low pressure

At low pressures, the behavior of gas flow changes significantly compared to atmospheric conditions. There are 2.5 main regimes (two different flow regimes and a “transitional” one) of gas flow relevant to vacuum systems:

- **Viscous (or continuum) flow:** At relatively high pressures (above ~1 mbar), collisions between residual gas molecules dominate the physical behavior. Flow is dominated by viscosity, and gases behave much like fluids. This flow regime matches our expectations of gas behavior in day-to-day lives in the atmosphere, where gasses rush to expand into free spaces.
- **Molecular (or free molecular) flow:** At very low pressures (below ~10^{-3} mbar), gas molecules rarely collide with each other and instead interact mainly with the walls of the vacuum chamber. In this regime, traditional fluid dynamics no longer apply, and gas transport is governed by the random motion of individual molecules. One important difference when in molecular flow is that residual gas molecules, because they are no longer pressed to fill empty space by collisions with other molecules, are much less likely

to enter small orifaces (which is leveraged when differential pumping is required) or move around corners.

- (**Transitional flow:** In the intermediate pressure range (~1 mbar to 10ˆ-3 mbar), both molecule-molecule and molecule-wall collisions are important. Flow characteristics are a mix of viscous and molecular behaviors.)

The transition between these regimes is described by the Knudsen number (Kn), which is the ratio of the mean free path of a molecule to a characteristic dimension (such as the diameter of a pipe). High Knudsen numbers ($Kn > 1$) indicate molecular flow, while low Knudsen numbers ($Kn < 0.01$) indicate viscous flow.

5.6.2 Vacuum Pumps

Vacuum pumps are “roughly” divided into low-vacuum, or roughing pumps, that operate in a viscous flow regime and can pump directly from atmospheric pressure, and high-vacuum pumps that operate in the molecular flow regime and typically require a minimum vacuum to operate.

5.6.2.1 Roughing pumps

Oil pumps Mercury diffusion pumps Scroll pumps Rotary vane pump Diaphragm pumps Roots pumps Getter pumps

5.6.2.2 High vacuum pumps

Turbos Ion pumps Cryo pumps

5.6.3 Material considerations

5.6.4 Flanges, gaskets, valves

5.6.5 Vacuum guages

5.7 Power components

5.7.1 High voltages and considerations

5.7.2 Mass spec power systems

UPS Transformer Power conditioner Chillers

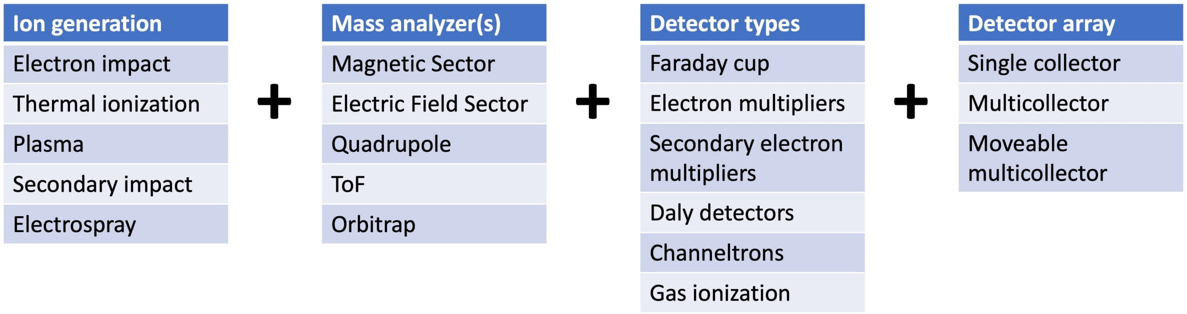
5.8 Computers

5.8.1 Data loops

6 Types of mass spectrometer

6.1 Overview

A variety of different types of mass spectrometers exist. In detail, the type of mass spectrometer is defined by the combination of an ion source, one more type of mass analyzer, and one or more type of detector.



Ion generation
Electron impact
Thermal ionization
Plasma
Secondary impact
Electrospray

+

Mass analyzer(s)
Magnetic Sector
Electric Field Sector
Quadrupole
ToF
Orbitrap

+

Detector types
Faraday cup
Electron multipliers
Secondary electron multipliers
Daly detectors
Channeltrons
Gas ionization

+

Detector array
Single collector
Multicollector
Moveable multicollector

Figure 6.1: *The combinations of ion sources, mass analyzers, and detector types/configurations are endless.* **ENDLESS.**

Different combinations of these three components will give you a different type of mass spectrometer. Since each type of mass spectrometer typically only has one type of ion source, we have organized this section at a high level by ion source, and then by type of mass analyzer or analyzers. We do not delve into detector arrays at this stage; while in practice the detector configuration matters for specific mass spectrometer applications, in terms of defining mass spectrometer 'types' this is the least important characteristic.

6.2 Thermal Ionization (TIMS)

Thermal ionization sources are basically only used in one type of mass spectrometer: a Thermal Ionization Mass Spectrometer, or TIMS. It's pretty straightforward: the ions are generated by thermal ionization, and then the ions are accelerated through a magnetic sector to achieve momentum to charge separation. Boom! It's that easy. The beautiful simplicity of the TIMS is why this was the first mass spectrometer to come into existence. In the geosciences, TIMS is most commonly used for high-precision and high-temperature geochronology (e.g., zircon U-Pb geochronology) and geochemistry (e.g., W isotopes). Before the advent of ICP-MS technology, TIMS was also commonly used for trace element analyses.

6.3 Electron Impact Source

Mass spectrometers with electron impact sources are used to analyze materials or samples that, upon being let into the mass spectrometer, are already in a gaseous state. The type of mass spectrometer that has an electron impact source is then defined by the type (or types) of mass analyzer the gaseous ions encounter after being accelerated away from the ion source.

6.3.1 Sector Field Mass Spectrometers

6.3.1.1 Static Volume Mass Spectrometers, Including Noble Gas Mass Spectrometers (NGMS)

Static volume mass spectrometers consist of an electron impact source and a magnetic sector mass analyzer. Importantly, with these mass spectrometers measurements are made ‘statically’, i.e., the volume of the mass spectrometer is not being pumped on by vacuum pumps during the analysis. Static volume mass spectrometers are very commonly utilized to analyze noble gas isotopes and other gases (e.g., N isotopes) extracted from solid materials where there is a finite, comparably small amount of gas that would be consumed too quickly if the mass spectrometer volume was being pumped on during the analysis. This type of instrument is commonly used for geochronology using noble gas systems (e.g., ^{40}Ar^{39}Ar).

6.3.1.2 Isotope Ratio Mass Spectrometers (IRMS)

6.3.2 Quadrupoles

6.3.2.1 Residual Gas Analyzers (RGAs)

Residual gas analyzers, or RGAs, are actually used in a variety of mass spectrometry laboratories for leak checking/testing: if atmosphere is somehow getting into your instrument via a leak somewhere in the vacuum system, RGAs can be used to detect it. However, RGAs can also be used for geochemical analyses involving gases when high sensitivity, precision, and mass resolution are not required. For example, this type of instrument is commonly used by the (U-Th)/He community to measure radiogenic ^{4}He analyses by isotope dilution.

6.3.2.2 Gas Chromatograph Mass Spectrometer

6.3.3 Electric Field Sector Instruments

6.3.3.1 Ion Traps

6.3.3.2 Orbitraps

6.4 Secondary Impact Source

6.4.1 Secodnary Ion Mass Spectrometers (SIMS and NanoSIMS)

6.4.2 TOF-SIMS

6.5 Accelerator Mass Spectrometers (AMS)

Accelerator mass spectrometers, or AMS, are undoubtedly the most complex type of mass spectrometers utilized in the geosciences. They can have secondary ion sources or laser ionization sources that ionize either solid or gaseous materials, and can have numerous magnetic sectors, quadrupoles, and electrostatic analyzers in various positions along the path through which ions traverse. The key or defining feature of an AMS, however, is the electrostatic tandem accelerator, which is a large (sometimes very large!) particle accelerator consisting of two stages.

The first stage of a tandem accelerator has a huge potential voltage across it that accelerates ions to very, very high kinetic energies. These high kinetic energy ions pass through a stripping material (e.g., gas or foil) that destroys molecules and also transforms the ions from negatively charged ions that originate from the source into positive ions, typically with high charge states. This is one if (if not the) most sensitive mass spectrometry techniques for measuring very rare isotopes, particularly when there is a major isotope of the same element that is many, many orders of magnitude more abundant. In the geosciences, AMS is most commonly used to measure cosmogenic radionuclides, which are isotopes generated in the atmosphere or in solid minerals by interactions with cosmic rays, such as ^{14}C, ^{10}Be, and ^{26}Al.

6.6 Inductively Copuled Plasma Source

6.6.1 Quadrupole ICPs

6.6.1.1 ICP-Q-MS

6.6.1.2 ICP-TOF

6.6.1.3 ICP-SF-MS (often just referred to as ICP-MS)

6.6.2 Tandem mass spectrometers (ICP-MS/MS)

6.6.2.1 Two mass analyzers + collision reaction cell

6.7 Electrospray Ionization

6.7.1 Orbitrap

6.7.2 Quadrupole

6.7.3 TOF

Part IV

Mass Spectrometer Design

7 Ion source design

8 Why ionization?

9 Metrics of ionization performance?

- Efficiency (molecules/ion) -> lower number better
- Selectivity: diversity of molecules that are ionized (tradeoff depends on application)
- Fragmentation: soft (molecular ions only) vs. hard (fragment ions produced) -> tradeoffs depending on application
- Adducts/molecular interferences made: H+ (EI), Ar+, O+ (in ICP), Na+ (in ESI)
- Intensity (beam "brightness". Brighter beams require physically larger instruments)
- Stability
- Collimation, energy distribution of ions

10 Types of ion sources

10.1 TIMS

10.1.1 Principles

10.1.2 Metrics

10.1.3 Uses/applications

10.1.4 Arcane knowledge/decision points

10.1.4.1 Filament choice

10.1.4.2 Ionization temperature

10.1.4.3 Ionization efficiency

10.1.4.4 Activators

10.1.4.5 Positive vs. negative ionization

10.1.4.6 Spikes

10.2 EI

10.2.1 Principles

10.2.2 Metrics

10.2.3 Uses/applications

10.2.4 Arcane knowledge/decision points

10.2.4.1 Noble gas

Time zero

Trap current

Accelerating voltage

Electron energy

Ion repeller

Trap voltage

Source plates

Half-plate

Z-plate

Octopole/flatopole

10.2.4.2 Stable isotopes

Electron energy

Linearity vs. sensitivity

Trap

Beam tightness, fragmentation patterns

Extraction

Sensitivity vs. linearity/recombination/scrambling

Source pressure

Sensivity vs linearity/recombination

Bellows pressure / capillary

Bleedout rate

R-plate

10.3 SIMS

10.3.1 Principles

10.3.2 Metrics

10.3.3 Uses/applications

10.3.4 Arcane knowledge/decision points

10.3.4.1 Primary ion beam (Cs vs O)

electronegratiivty.where you are on the periodic table

Cs reactions/implantation

10.3.4.2 Beam intensity

10.3.4.3 Beam size

10.3.4.4 Beam energy density

10.3.4.5 Ion microprobe vs ion microscope

10.4 ICP

10.4.1 Principles

10.4.2 Metrics

10.4.3 Uses/applications

10.4.4 Arcane knowledge/decision points

10.5 MALDI

10.5.1 Principles

10.5.2 Metrics

10.5.3 Uses/applications

10.5.4 Arcane knowledge/decision points

10.6 ESI

10.6.1 Principles

10.6.2 Metrics

10.6.3 Uses/applications

10.6.4 Arcane knowledge/decision points

10.7 CI

10.7.1 Principles

10.7.2 Metrics

10.7.3 Uses/applications

10.7.4 Arcane knowledge/decision points

10.7.4.1 Type of chemical ionization

(acetate, iodide, or water (PTR))

Atmospheric pressure drift tube

EESI

Temperature stability

Ionization pressure

Fragmentation tradeoffs

11 Mass analyzer design

What's the difference between an analyzer and a filter? We don't know.

Short description of advantages and disadvantages of each type.

11.1 Magnetic sectors

Quick recap of why we need magnets and the dispersion equation. Lorentz force.

11.1.1 History of magnetic sector geometries

Dempster, sector field, extended geometry. Focal planes.

11.1.2 Extended geometry magnetic sector in practice

Dispersion, focal plane geometry.

11.2 Electrostatic Analyzers (ESA)

Why use an ESA instead of a magnet? Before or after magnet? Why is it so often seen on ICPs and less often (or even not at all!) on a TIMS. Reference Coulomb force, a figure of an ion traversing a ESA.

Advantage is that you can change a voltage quickly (nanoseconds), for instance to deflect a beam.

11.3 Quadrupole Mass Analyzers

Quadrupoles are a dynamic mass analyzer. Quickly changing voltages. Radio frequency.

Hexapoles and Octopoles. RF multipoles in general.

Rod shapes and resulting EM field lines. Compromises with number and shape of rods.

Advantages: no moving parts, very fast, reliable, inexpensive (see also, vacuum systems and requirements). Disadvantages: One m/z out the back end at a time. Throughput can be low.

Stability triangle figure.

Lots of math with funny symbols.

11.4 Time of flight mass analyzer (TOF)

Some history. Space applications. Nanoparticle and environmental applications.

Geometries: reflection plates or not.

Notch filters. If you have oxygen, you have to notch it because it overwhelms everything else.

Simultaneous collection of all ionized species regardless of mass.

Disadvantages: Much less sensitive for low-z species. Lower sensitivity than quadrupole, also more expensive. Advantages: really fast, very small (fits on a benchtop), suited for imaging applications, portable applications, and extraterrestrial applications.

11.5 Accelerator Mass Spectrometer (AMS)

Large, expensive instruments, very high voltages. Contains several of the mass analyzers mentioned above, plus more components.

11.6 Orbitrap mass analyzer

Max can clean this up later. Thanks Max!

11.7 Ion trap mass analyzer

Stephen can discuss advantages and disadvantages here.

12 Detector design

12.1 Overview

What are we detecting, and why?

Why you would choose to use one detector over another?

- beam size
- statistics
- detector size
- other considerations (e.g., can't use scintillators for NGMS)

12.2 Faraday Detectors

12.2.1 Faraday Cup Hardware

12.2.2 Amplifier Electronics

- RTIAs
- CTIAs

12.3 Electron Multipliers

12.3.1 Operating Mode and Electronics

- Ion Counting
- Analog

12.3.2 Discrete Dynode Multipliers

12.3.3 Channeltrons

12.3.4 Daly Detectors

12.4 Other Exotic Detector Type

CCDs Gas ionization detectors Other scintillation detectors

13 Vacuum systems

Part V

Analytical Considerations

14 Baselines

15 Peak Tails and Abundance Sensitivity

References

Bleakney, Walker. 1929. “A New Method of Positive Ray Analysis and Its Application to the Measurement of Ionization Potentials in Mercury Vapor.” *Physics Reviews* 34 (157).

Date, Alan R., and Alan L. Gray. 1981. “Plasma Source Mass Spectrometry Using an Inductively Coupled Plasma and a High Resolution Quadrupole Mass Filter.” *Analyst* 106: 1255–67. https://doi.org/10.1039/AN9810601255.

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Fenn, John B, Matthias Mann, Chin Kai Meng, Shek Fu Wong, and Craige M Whitehouse. 1990. “Electrospray Ionization–Principles and Practice.” *Mass Spectrometry Reviews* 9 (1): 37–70.

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Wang, Meng, W. J. Huang, F. G. Kondev, G. Audi, and S. Naimi. 2021. “The AME 2020 Atomic Mass Evaluation (II). Tables, Graphs and References*.” *Chinese Physics C* 45 (3): 030003. https://doi.org/10.1088/1674-1137/abddaf.

Yergey, Alfred L., and A. Karl Yergey. 1997. “Preparative Scale Mass Spectrometry: A Brief History of the Calutron.” *Journal of the American Society for Mass Spectrometry* 8 (9):

943–53. https://doi.org/https://doi.org/10.1016/S1044-0305(97)00123-2.

Part VI

Isotope Systems

16 Ar/Ar

17 U/Pb

18 (U–Th)/He

19 Re-Os

Sample text here

Part VII

Interpreting Data

20 Statistics for Mass Spectrometer Jockeys

References

Bleakney, Walker. 1929. "A New Method of Positive Ray Analysis and Its Application to the Measurement of Ionization Potentials in Mercury Vapor." *Physics Reviews* 34 (157).

Date, Alan R., and Alan L. Gray. 1981. "Plasma Source Mass Spectrometry Using an Inductively Coupled Plasma and a High Resolution Quadrupole Mass Filter." *Analyst* 106: 1255–67. https://doi.org/10.1039/AN9810601255.

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Nier, Alfred. 1947. "A Mass Spectrometer for Isotope and Gas Analysis." *The Review of Scientific Instruments* 18 (6).

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Wang, Meng, W. J. Huang, F. G. Kondev, G. Audi, and S. Naimi. 2021. "The AME 2020 Atomic Mass Evaluation (II). Tables, Graphs and References*." *Chinese Physics C* 45 (3): 030003. https://doi.org/10.1088/1674-1137/abddaf.

Yergey, Alfred L., and A. Karl Yergey. 1997. "Preparative Scale Mass Spectrometry: A Brief History of the Calutron." *Journal of the American Society for Mass Spectrometry* 8 (9):

943–53. https://doi.org/https://doi.org/10.1016/S1044-0305(97)00123-2.

A Contributing to Mass Spec Academy

You can contribute to Mass Spec Academy by writing new material or editing existing content. The best way to do this and see how your new content will look is to use the Quarto publishing system and download and submit content through our GitHub repository.

A.1 Overview

We are using Quarto to render our instructional materials as user-friendly web and pdf documents. It's free and open source, and it's designed for open science projects like ours. Quarto lets you use all the components of a traditional academic manuscript or textbook, like text organized into chapters and sections, figures and tables with captions, equations with numbers, and references to cited work and to all those chapters/sections/equations/figures.

But wait, there's more: you can add movies, links to content from other chapters, code that drives computations and visualizations, callout blocks (like the topical side-boxes you see in textbooks, but with more options), and much else. Quarto renders this content both as a nice-looking webpage with lots of navigational features, and as a pdf file.

You can find nice examples of Quarto-authored books here:

- R for Data Science (2e)
- Geocomputation with Python
- Causal Inference in R

A.2 Software Installation

To author new or edit existing content on your computer, you'll need to install some software. This tutorial will help you get set up — please skip installs for any software you already have. You will need:

1. Conda to organize and manage our code tools
2. VSCode to write content
3. The Quarto Command Line Interface (CLI)
    - and the Quarto VS Code extension

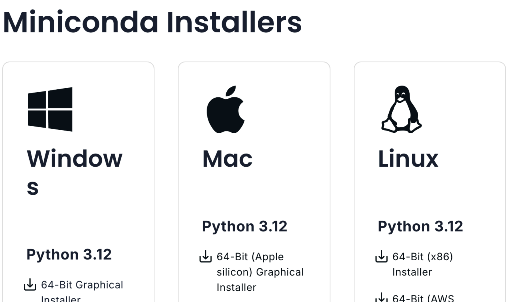
4. GitHub Desktop as a user-friendly interface with GitHub (optional)

A.2.1 Step 1: (Mini)conda

We'll use conda to keep track of all the smaller software packages that get used to create our source material. If you have already downloaded Anaconda for some previous data/science work, then great, you're all set! If not, you can download a smaller version without all the extra tools we won't use, called Miniconda.

This is the most involved install, so we're doing it first. The others are easy. Go to https://www.anaconda.com/download/success, scroll down past the Anaconda installers, and choose the Miniconda installer for your operating system. There is a Python version next to this, but don't worry about it, there's no Python involved here. If you're still reading this text, you probably want the "Graphical Installer" option. Note that *DO NOT* need to send your email address to anaconda.com to download or use this.

Screenshot of anaconda.com/download/success



More detailed instructions for Miniconda installation are here for each OS under "Basic install instructions." In short, the instructions are to choose an install path with no spaces (the default is a good idea).

For **Windows**, you'll also want to

- install for "Just Me" instead of "All Users,"

- create shortcuts (selected by default) for Anaconda Prompt packages, and
- do <u>not</u> "Add Miniconda3 to my PATH variable"

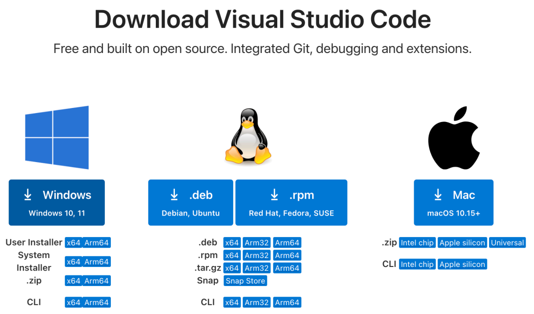
That wasn't so bad, right?

A.2.2 Step 2: VS Code

You can use any editor you want for Quarto, but this tutorial will show you how to set up Microsoft Visual Studio (VS) Code. It's free, "built from open source," and it's widely used.

You can consider yourself a hacker once you download VS Code from https://code.visualstudio.com/download. If you don't know which of the buttons to choose for your operating system, then click on the big button. VS Code is smallish (< 200 MB download, < 500 MB disk space).

Screenshot of code.visualstudio.com/download



Download Visual Studio Code

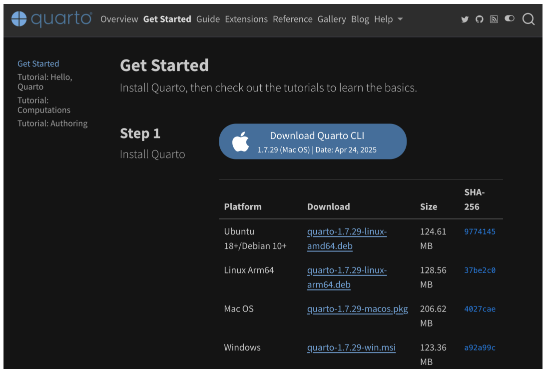
Free and built on open source. Integrated Git, debugging and extensions.

Install VSCode and follow the prompts. We'll add extensions and additional components later.

A.2.3 Step 3: Quarto CLI

Download the Quarto Command Line Interface (CLI) from https://quarto.org/docs/get-started/ for your operating system. Install and follow the installer instructions. This is another small-ish ~200 MB installer. To update Quarto when a new version is released, you'll need to download the new installer from this website and install it again.

Screenshot of quarto.org/docs/get-started/



Get Started
Tutorial: Hello, Quarto
Tutorial: Computations
Tutorial: Authoring

Get Started

Install Quarto, then check out the tutorials to learn the basics.

Step 1

Install Quarto

Download Quarto CLI
1.7.29 (Mac OS) | Date: Apr 24, 2025

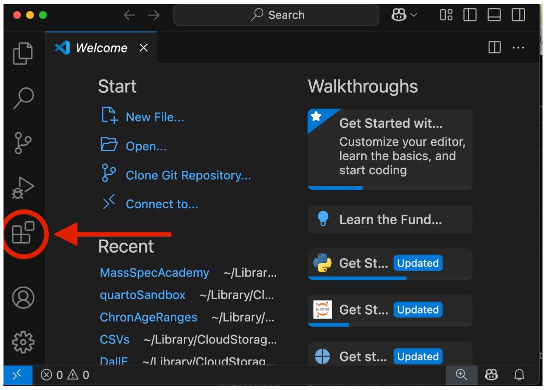
Platform	Download	Size	SHA-256
Ubuntu 18+/Debian 10+	quarto-1.7.29-linux-amd64.deb	124.61 MB	9774145
Linux Arm64	quarto-1.7.29-linux-arm64.deb	128.56 MB	37be2c0
Mac OS	quarto-1.7.29-macos.pkg	206.62 MB	4027cae
Windows	quarto-1.7.29-win.msi	123.36 MB	a92a99c

Quarto is what will turn the text we write in VS Code into content that looks pretty on the web, both on desktops and on mobile screens, and a pdf.

A.2.3.1 Step 3A: Add the Quarto VS Code Extension

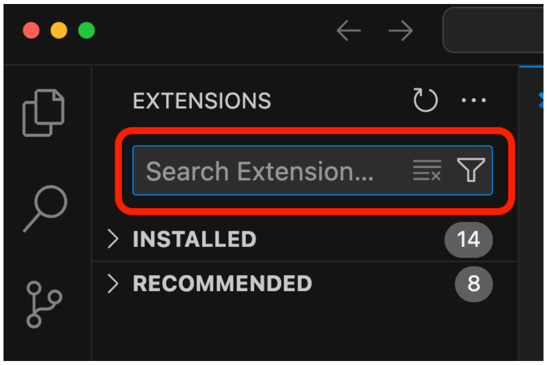
Open VS Code and then find the Extensions button on the left sidebar. It looks like some squares with the NE square levitating.

Screenshot of quarto.org/docs/get-started/



Then, click inside the Search bar and type "Quarto."

Screenshot of quarto.org/docs/get-started/



You'll see the Quarto extension up first. Click on the extension to open an information window, then click the Install button on this window. You'll need the Quarto CLI installed in order to make the VS Code extension work.

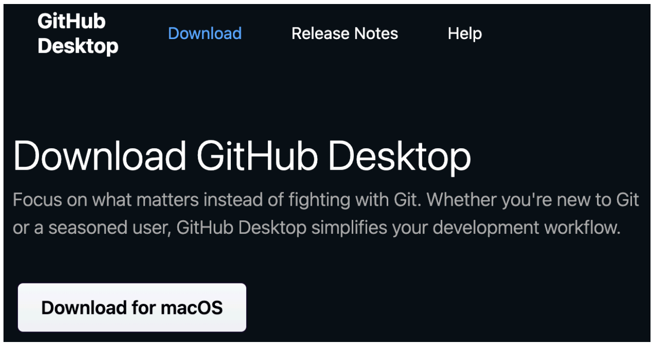
The Quarto extension lets VS Code recognize your Quarto-formatted files, then makes it easier to edit those files. It colors your text based on its purpose (headers, links, images, code), lets you drag and drop image files into documents, and provides a preview of your work with the click of a button.

A.2.4 Step 4: GitHub Desktop

We will use the version control software Git, and we will host all of our content, like writing and figures, on GitHub.com. All current and previous versions of content on GitHub are publicly available through the GitHub.com website. Additionally, GitHub serves the website version of our project, for free, through GitHub Pages. Changes to the project that are pushed up to GitHub repository are automatically rendered to the website. If this makes no sense now, don't worry.

The easiest way to download and install Git and to start working with our GitHub repository is to download the GitHub Desktop app from https://desktop.github.com/download/. GitHub knows what operating system you're using, and probably what you ate for lunch last Wednesday, so just click the button to download.

Screenshot of desktop.github.com/download



Download GitHub Desktop

Focus on what matters instead of fighting with Git. Whether you're new to Git or a seasoned user, GitHub Desktop simplifies your development workflow.

You will need to sign in with a GitHub.com username and password. Create one if you don't already — sorry, this is the only new login you'll need for this project.

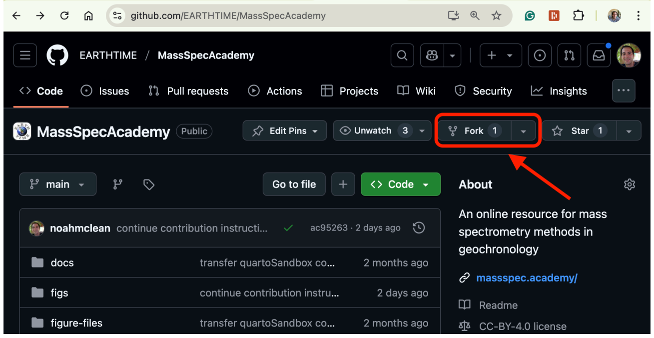
A.3 Getting started!

Now that you've installed all the software you need, we will download the current version of the project onto your computer using GitHub Desktop, install the packages it depends on using conda, and then open it for editing in VS Code.

A.3.1 1. Fork the MassSpecAcademy GitHub repository

Sign in to GitHub.com with your username and password, then navigate to https://github.com/EARTHTIME/MassSpecAcademy. Find and click the 'Fork' button at the top right of the screen.

Screenshot of github.com/EARTHTIME/MassSpecAcademy



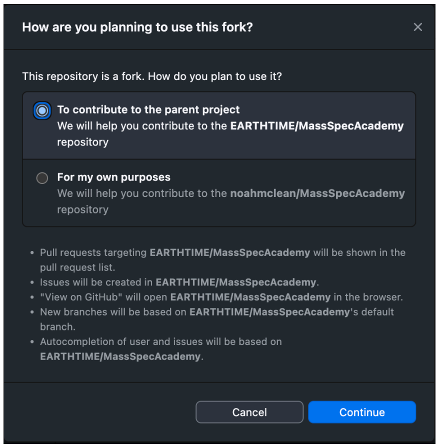
An online resource for mass spectrometry methods in geochronology

Press the Green "Create Fork" button at the bottom left of the next screen to create your own copy of the MassSpecAcademy repository on your own GitHub account. Now open the GitHub Desktop App, click the sign in with your GitHub username and password, and then from the "File" menu, choose "Clone Repository…"

In the window that pops up, find your new personal copy of the MassSpecAcademy repository in the list of repositories from GitHub.com. This repository will be a single folder with all the files and subfolders of Mass Spec Academy inside it. Choose a Local Path for this folder (the default is usually good), then click the blue Clone button.

Next, a window from GitHub Desktop will pop up and ask you how you want to use the repository. You want to contribute to the parent project, so keep the radio button in its top position and hit Continue.

Screenshot of popup: how do you want to use this repository?



How are you planning to use this fork?

This repository is a fork. How do you plan to use it?

● **To contribute to the parent project**
We will help you contribute to the **EARTHTIME/MassSpecAcademy** repository

○ **For my own purposes**
We will help you contribute to the **noahmclean/MassSpecAcademy** repository

- Pull requests targeting **EARTHTIME/MassSpecAcademy** will be shown in the pull request list.
- Issues will be created in **EARTHTIME/MassSpecAcademy**.
- "View on GitHub" will open **EARTHTIME/MassSpecAcademy** in the browser.
- New branches will be based on **EARTHTIME/MassSpecAcademy**'s default branch.
- Autocompletion of user and issues will be based on **EARTHTIME/MassSpecAcademy**.

You now have a copy of Mass Spec Academy on your own computer!

A.3.2 2. Create a new branch for your edits

A.3.2.1 Quick workflow overview:

There are now two versions of the MassSpecAcademy repository on GitHub: the main project repository owned by EARTHTIME and the forked copy of the repository that you now own. The main project repository on GitHub is called “upstream” and the one attached to your GitHub account is called “origin.” We also just used GitHub Desktop to make a local copy of your fork on your computer. This local copy is a little sandbox where you can change anything you want — you could mess up your local repository and/or your forked repository on GitHub without affecting the larger project or its web presence.

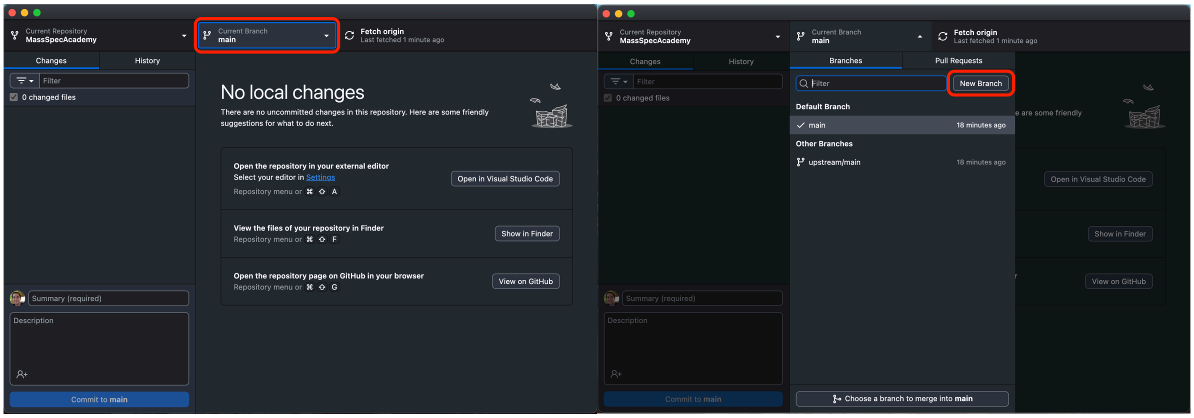
The feature branch we’re about to create in your forked GitHub repository will be a place that you create and edit your Mass Spec Academy content. You can create a new branch for each contribution you plan to make. For instance, you could make a branch for a project like “Start TIMS applications chapter” or “Edit background sections.” You’ll use GitHub desktop to package up each small batch of edits as a “commit” and to synchronize the edits on your local computer with your forked GitHub repository online.

When you’re at a place with your project where you want to merge your edits with the “upstream” main repository, you will create a Pull Request using the instructions below. This alerts the project maintainers (currently Stephen Cox and Noah McLean) that your content is ready. The maintainers can review your content, make suggestions or edits with the opportunity for a group discussion, and then merge your content into the main project. The merge will become visible to everyone else working on the project, and it will automatically update the website and pdf document. Now you can make a new branch for your next set of edits!

A.3.2.2 Create your new feature branch.

In GitHub Desktop, find the “Branches” dropdown menu in the middle of the top of the app window. Click anywhere in the button to make the dropdown menu appear, and click the “New Branch” button at its top right.

Type in a name for your feature branch that describes the work you’re about to do, or just “testing” if you want to try it out. Hit enter to create your new branch, and you’re off to the races.



No local changes

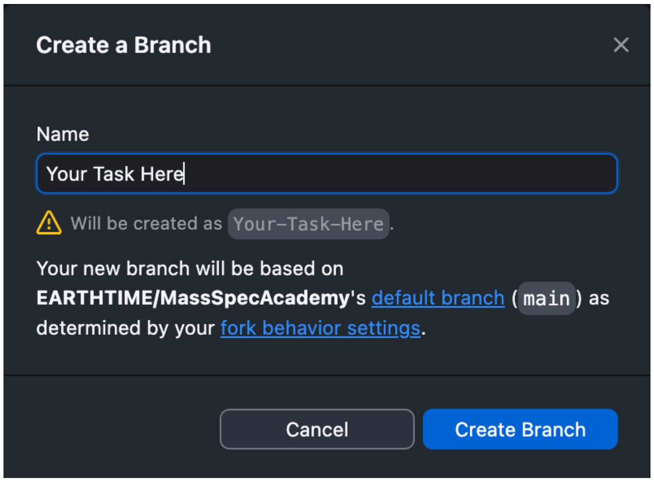
There are no uncommitted changes in this repository. Here are some friendly suggestions for what to do next.

Open the repository in your external editor
Select your editor in Settings
Repository menu or ⌘ ⇧ A

View the files of your repository in Finder
Repository menu or ⌘ ⇧ F

Open the repository page on GitHub in your browser
Repository menu or ⌘ ⇧ G

GitHub Desktop new branch window screenshot



Name

Your Task Here

Will be created as `Your-Task-Here`.

Your new branch will be based on **EARTHTIME/MassSpecAcademy**'s default branch (`main`) as determined by your fork behavior settings.

As long as the name of your branch is showing under the “Current Branch” button on GitHub Desktop, your edits will belong to this branch.

A.3.3 3. Use conda to download dependencies

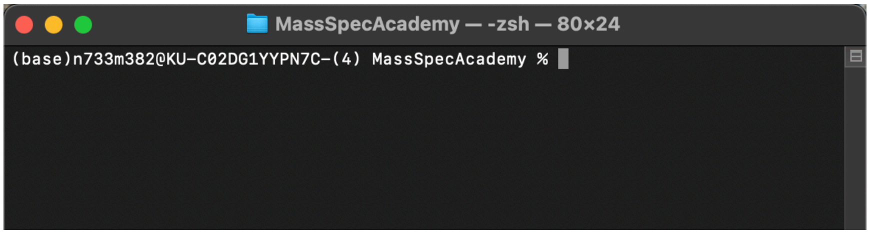
In order to reproduce the Mass Spec Academy website and run all of its code blocks, like the ones planned for its data and statistics chapters, you’ll need to install Python and some packages. This is easy with conda.

On a Mac, navigate in Finder to your new MassSpecAcademy folder that contains our local git repository. Then right-click on the MassSpecAcademy folder and, down the list of options, choose “New Terminal At Folder”.

On Windows, navigate in Windows Explorer to the MassSpecAcademy folder you created with GitHub Desktop. Copy the folder location from the address bar at the top of Windows Explorer. Now open the Anaconda Command Prompt application that was created when you installed Miniconda – it should be listed beside all your other applications, available from your Windows button. Type `cd "` (that is the letter `cd`, a space, then a double quotes), then paste in the path you copied, then type a second `"` to close the quotes. Hit the enter key.

On Windows or a Mac, you should now see a blinking cursor to the right of some text that starts with `(base)` and ends with `MassSpecAcademy`, the name of your current folder, like this:

Terminal screenshot from the start of making a new conda environment



```
(base)n733m382@KU-C02DG1YYPN7C-(4) MassSpecAcademy %
```

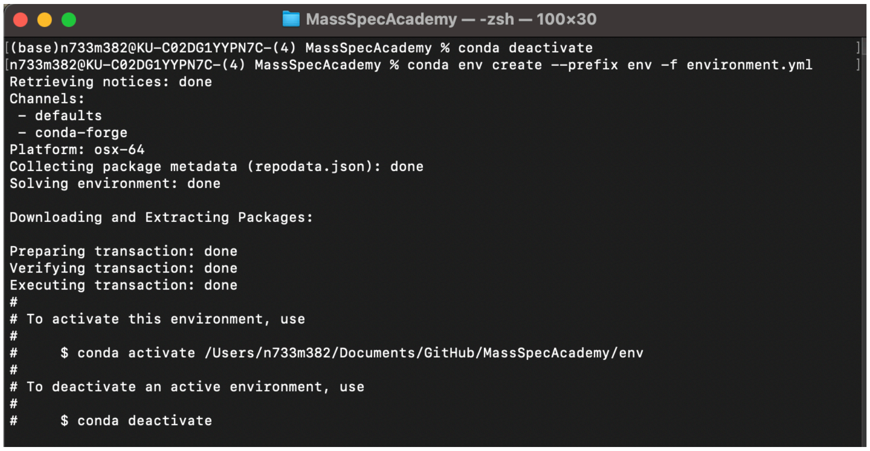
First, type `conda deactivate`, and hit enter. The `(base)` at the beginning of the line should disappear.

Now, copy and paste this text at that blinking cursor, then hit enter:

```
conda env create --prefix env -f environment.yml
```

When you hit enter, conda will think some and tell you what it is up to, i.e., … “Retrieving notices,” “Solving environment,” “Collecting package metadata,” etc. After ten or twenty seconds, conda will output a few lines of instructions for activating and deactivating your new environment. You can ignore these — you’re done with conda and the command line for now. Your terminal should look something like this:

End of conda new environment from terminal



MassSpecAcademy — -zsh — 100×30

```
[(base)n733m382@KU-C02DG1YYPN7C-(4) MassSpecAcademy % conda deactivate                               ]
[n733m382@KU-C02DG1YYPN7C-(4) MassSpecAcademy % conda env create --prefix env -f environment.yml     ]
Retrieving notices: done
Channels:
 - defaults
 - conda-forge
Platform: osx-64
Collecting package metadata (repodata.json): done
Solving environment: done

Downloading and Extracting Packages:

Preparing transaction: done
Verifying transaction: done
Executing transaction: done
#
# To activate this environment, use
#
#     $ conda activate /Users/n733m382/Documents/GitHub/MassSpecAcademy/env
#
# To deactivate an active environment, use
#
#     $ conda deactivate
```

A.3.4 3. Open VS Code

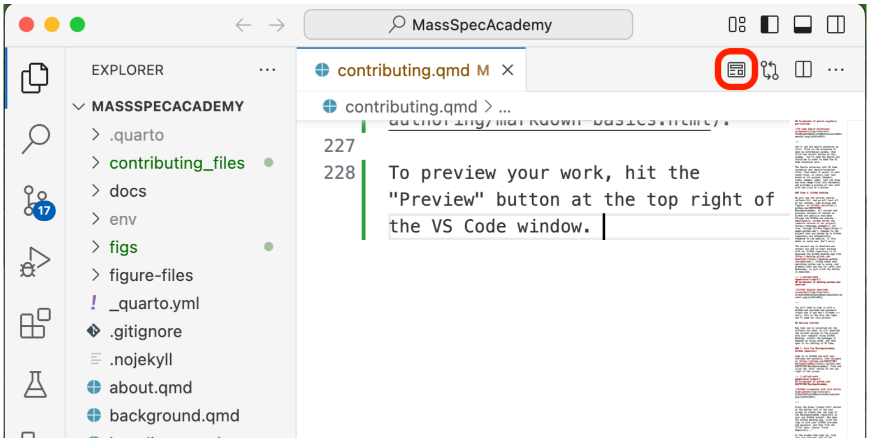
Open the VS Code application you downloaded and installed earlier. From the File menu, select "Open Folder…" and then navigate to the "MassSpecAcademy" folder that contains the forked GitHub repository you created with GitHub Desktop. It's probably in your Documents/GitHub folder. Select the MassSpecAcademy folder and then hit the Open button to open the folder.

You're in! You'll see a panel to the left with a file directory for the whole repository. You can double-click a file to open it for editing, or create a new Quarto .qmd file (right-click and choose "New File", use a button near the top of the panel, or from the "File" menu).

There's lots more on authoring Quarto content at https://quarto.org/docs/authoring/markdown-basics.html.

To preview your work, hit the "Preview" button at the top right of the VS Code window:

VS Code screenshot with Preview button highlighted



```
To preview your work, hit the
"Preview" button at the top right of
the VS Code window.
```

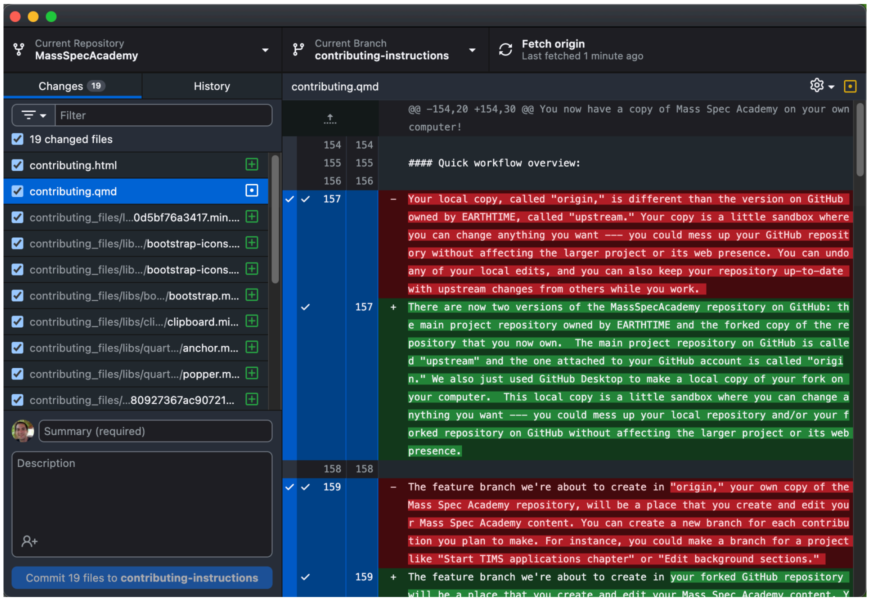
A preview panel will open on the right hand side of VS Code that you can resize to make readable. Another panel will open at the bottom that contains an integrated terminal window with output from Quarto about what it's doing.

If you've previewed a file that is already part of the website, then you will wait a minute, then see an interactive preview of the entire website. If you have previewed a new .qmd file that is not yet attached to the website navigation, you will see a preview of this page only. Command or control-click the http://localhost:XXXX/ link that appears in the terminal window or copy the same text from the top of the preview window and paste it into a browser to preview your content in a web browser. You can hit preview as often as you like to preview your changes and make sure your content is rendering correctly.

A.3.5 4. Commit your edits on GitHub Desktop

When you've hit a natural stopping place, like completing some writing or editing a section, or you're wrapping up and taking a long break, then it's time to commit your work. Open GitHub Desktop and you'll find that the left-hand panel titled "Changes" contains a list of all the files you've added, modified, or deleted. Each file will have a check box next to it, checked by default. The larger right-hand panel will show you all the changes you've made, with new content in green and deleted content in red.

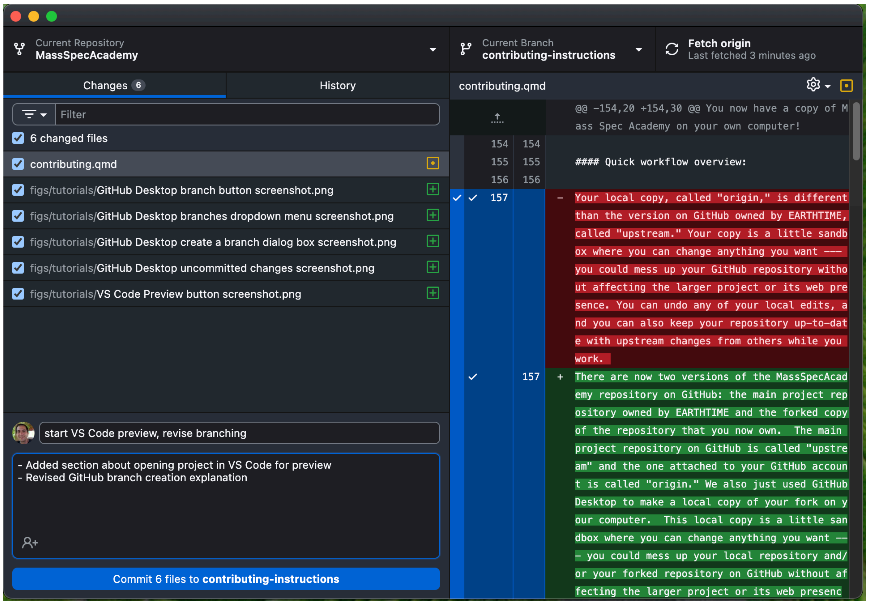
GitHub Desktop screenshot with uncommitted changes



```
@@ -154,20 +154,30 @@ You now have a copy of Mass Spec Academy on your own computer!
154 154
155 155  #### Quick workflow overview:
156 156
157      - Your local copy, called "origin," is different than the version on GitHub owned by EARTHTIME, called "upstream." Your copy is a little sandbox where you can change anything you want --- you could mess up your GitHub repository without affecting the larger project or its web presence. You can undo any of your local edits, and you can also keep your repository up-to-date with upstream changes from others while you work.
    157  + There are now two versions of the MassSpecAcademy repository on GitHub: the main project repository owned by EARTHTIME and the forked copy of the repository that you now own.  The main project repository on GitHub is called "upstream" and the one attached to your GitHub account is called "origin." We also just used GitHub Desktop to make a local copy of your fork on your computer.  This local copy is a little sandbox where you can change anything you want --- you could mess up your local repository and/or your forked repository on GitHub without affecting the larger project or its web presence.
158 158
159      - The feature branch we're about to create in "origin," your own copy of the Mass Spec Academy repository, will be a place that you create and edit your Mass Spec Academy content. You can create a new branch for each contribution you plan to make. For instance, you could make a branch for a project like "Start TIMS applications chapter" or "Edit background sections."
    159  + The feature branch we're about to create in your forked GitHub repository will be a place that you create and edit your Mass Spec Academy content. Y
```

Next, find the commit message area in the bottom left of the GitHub Desktop window. In the "Summary" bar, write a short summary of your edits (ideally < 50 characters), like "Add explanation of work function for TIMS." In the the "Description" box below, you can optionally leave a concise explanation of your edits. The commit message will be preserved alongside your edits and will help everyone understand your proposed changes and find where/when content was edited in case changes need to be reverted.

GitHub Desktop example commit message



☑ 6 changed files

- ☑ contributing.qmd
- ☑ figs/tutorials/GitHub Desktop branch button screenshot.png
- ☑ figs/tutorials/GitHub Desktop branches dropdown menu screenshot.png
- ☑ figs/tutorials/GitHub Desktop create a branch dialog box screenshot.png
- ☑ figs/tutorials/GitHub Desktop uncommitted changes screenshot.png
- ☑ figs/tutorials/VS Code Preview button screenshot.png

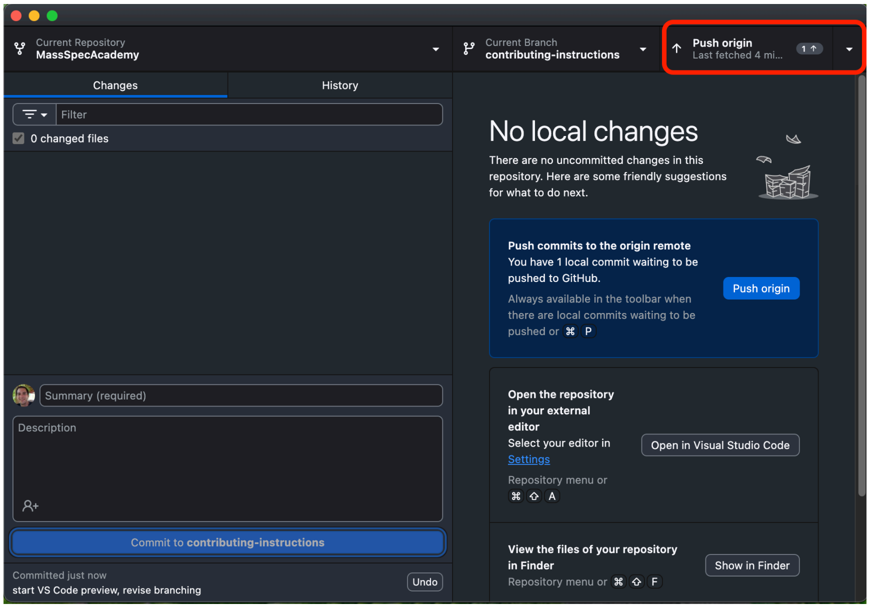
start VS Code preview, revise branching

- Added section about opening project in VS Code for preview
- Revised GitHub branch creation explanation

```
@@ -154,20 +154,30 @@ You now have a copy of M
ass Spec Academy on your own computer!
154 154
155 155    #### Quick workflow overview:
156 156
157      - Your local copy, called "origin," is different
           than the version on GitHub owned by EARTHTIME,
           called "upstream." Your copy is a little sandb
           ox where you can change anything you want ---
           you could mess up your GitHub repository witho
           ut affecting the larger project or its web pre
           sence. You can undo any of your local edits, a
           nd you can also keep your repository up-to-dat
           e with upstream changes from others while you
           work.
    157  + There are now two versions of the MassSpecAcad
           emy repository on GitHub: the main project rep
           ository owned by EARTHTIME and the forked copy
           of the repository that you now own.  The main
           project repository on GitHub is called "upstre
           am" and the one attached to your GitHub accoun
           t is called "origin." We also just used GitHub
           Desktop to make a local copy of your fork on y
           our computer.  This local copy is a little san
           dbox where you can change anything you want --
           - you could mess up your local repository and/
           or your forked repository on GitHub without af
           fecting the larger project or its web presenc
```

When you're done, hit the blue "Commit" button at the bottom left of the GitHub Desktop window. Your changes have now been wrapped up as a commit in the local version of your MassSpecAcademy repository on your computer. To synch the commit with your forked GitHub repository online, called "origin", click the "Push origin" button at the top right of the GitHub Desktop window.

GitHub Desktop screenshot of commit ready to push to origin



No local changes

There are no uncommitted changes in this repository. Here are some friendly suggestions for what to do next.

Push commits to the origin remote

You have 1 local commit waiting to be pushed to GitHub.

Always available in the toolbar when there are local commits waiting to be pushed or ⌘ P

Open the repository in your external editor

Select your editor in Settings

Repository menu or ⌘ ⇧ A

View the files of your repository in Finder

Repository menu or ⌘ ⇧ F

Committed just now

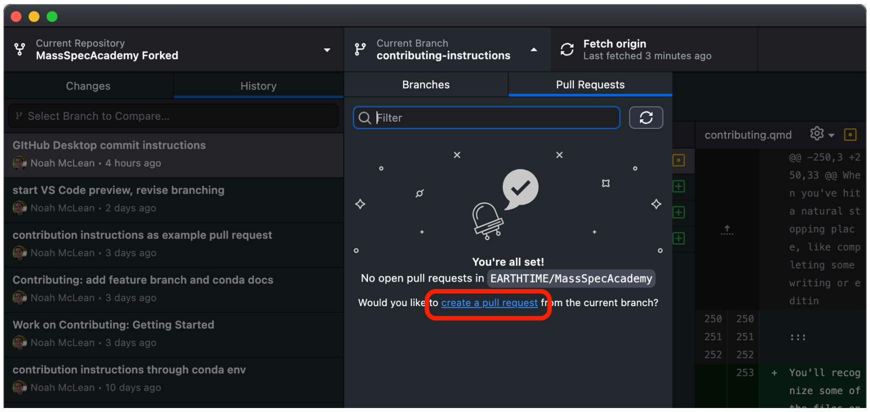
start VS Code preview, revise branching

A.3.6 5. Create a Pull Request

At any time after you've made the first commit to your new branch, you can open a **draft pull request**, which alerts everyone working on the upstream EARTHTIME/MassSpecAcademy repository that you have some changes you'd like to eventually merge into the main repository. You can keep making commits to your branch, which then get added to the draft pull request. When the branch is ready, you'll indicate that your work is "Ready for review." Stephen and Noah will make sure it doesn't break anything, then merge it into the main repository, which will update the website automatically.

To create a draft pull request, click on the "Current Branch" dropdown button at the center top of the GitHub Desktop window. There are two tabs for the dropdown, "Branches" and "Pull Requests." Click the "Pull Requests" tab to see a blue text link that offers to open a new pull request for you.

GitHub Desktop screenshot of the pull requests tab on the “Current Branch” dropdown



GItHub Desktop commit instructions
Noah McLean • 4 hours ago

start VS Code preview, revise branching
Noah McLean • 2 days ago

contribution instructions as example pull request
Noah McLean • 3 days ago

Contributing: add feature branch and conda docs
Noah McLean • 3 days ago

Work on Contributing: Getting Started
Noah McLean • 3 days ago

contribution instructions through conda env
Noah McLean • 10 days ago

You're all set!

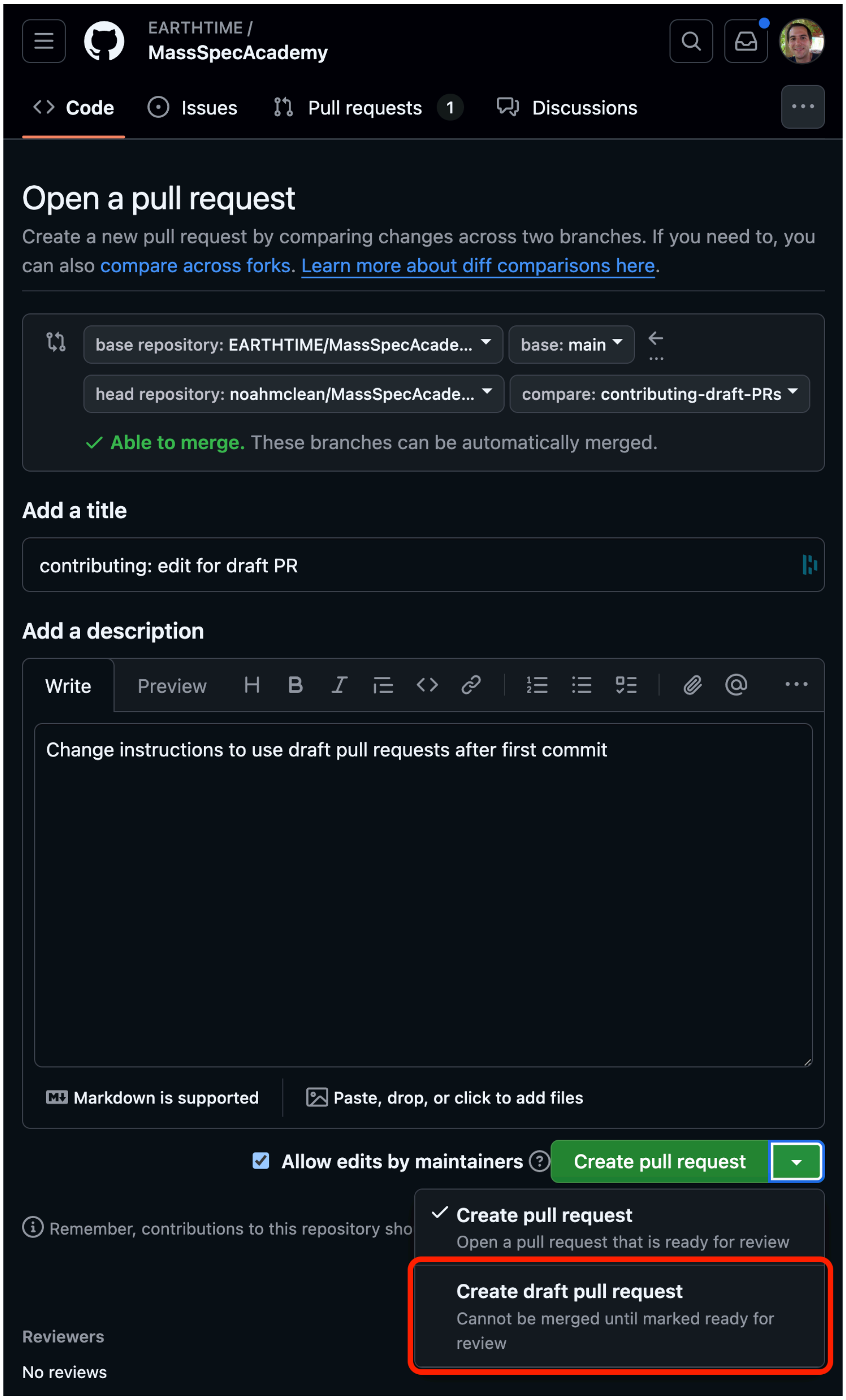
No open pull requests in `EARTHTIME/MassSpecAcademy`

Would you like to create a pull request from the current branch?

Clicking the blue link to “create a pull request” will open a new browser tab at the EARTHTIME/MassSpecAcademy repository. If you don’t see the little spaceship drawing, you can also go to the main menu at the top of the screen, click “Branch”, then “View Pull Request on GitHub.”

The EARTHTIME/MassSpecAcademy GitHub.com page will be pre-populated with all the right selections for creating a new pull request from the branch in your forked repository that you’ve been working on. Enter a good summary and description for what you plan to contribute in this pull request (e.g., “update SIMS figures” or “add chapter on calutron history”). Then click the dropdown arrow next to the green “Create Pull Request” button and choose “Create draft pull request”:

ℹ GitHub website screenshot of creating a draft pull request



Open a pull request

Create a new pull request by comparing changes across two branches. If you need to, you can also compare across forks. Learn more about diff comparisons here.

base repository: EARTHTIME/MassSpecAcade...

base: main

head repository: noahmclean/MassSpecAcade...

compare: contributing-draft-PRs

✓ Able to merge. These branches can be automatically merged.

Add a title

contributing: edit for draft PR

Add a description

Change instructions to use draft pull requests after first commit

Markdown is supported

Paste, drop, or click to add files

☑ Allow edits by maintainers

✓ Create pull request
Open a pull request that is ready for review

Create draft pull request
Cannot be merged until marked ready for review

Remember, contributions to this repository sho

Reviewers

No reviews

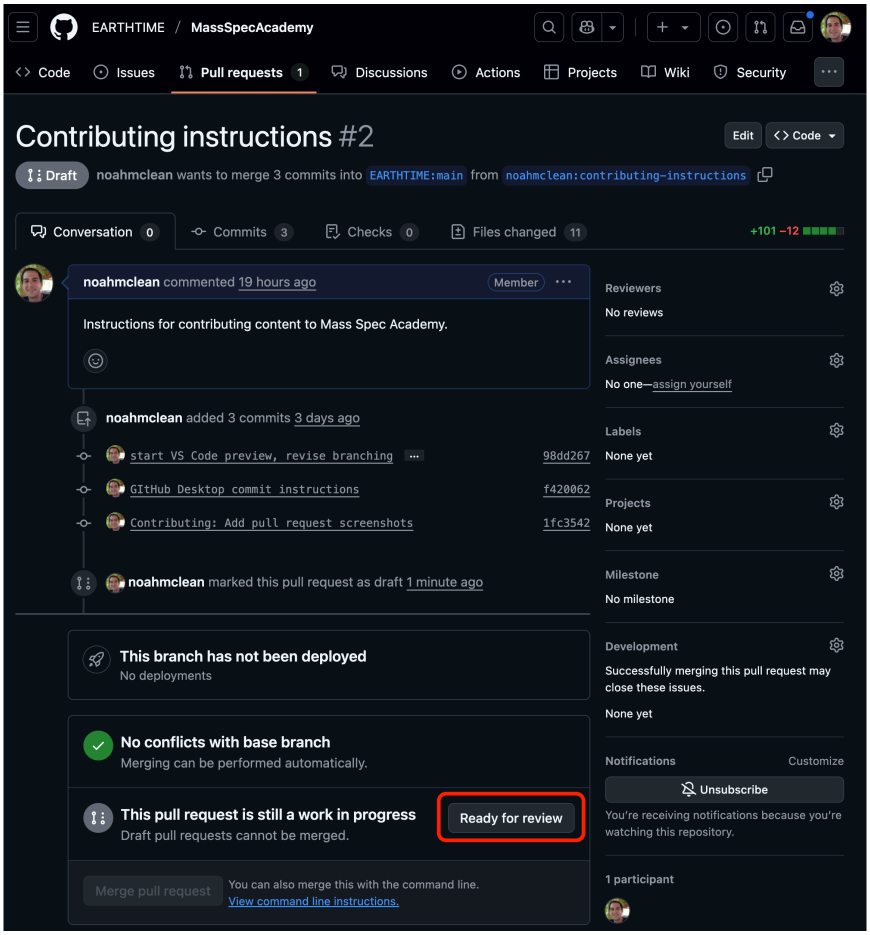
You can go to https://github.com/EARTHTIME/MassSpecAcademy/pulls to see all the other open draft pull requests, which represent others' in-progress contributions. Click the link for a pull request to read the commit messages and see how each project is progressing, and click a link to a commit to view its contents. This way, even though everyone is working on their own personal copy of the code on their own computer, you can get a sense of what others are doing. The pull requests page on the central repository linked above also serves as a discussion page – you can leave comments, ask questions, and make suggestions here, and the author will be notified by with an email from GitHub.

A.4 Get contributing!

Now that you have all the software installed and infrastructure in place, you should be able to add and edit content using the Quarto plugin for VS Code, previewing the results in a browser window as you write. When you've completed a task or chunk of text, you can commit those changes to your local repository on GitHub Desktop and push those changes to your online forked repository on GitHub.com.

When your content is ready to be added to the upstream EARTHTIME/MassSpecAcademy repository and the website, then change your draft pull request to a submitted pull request, which tells Stephen and Noah it's time to review and merge your branch. To do this, go to https://github.com/EARTHTIME/MassSpecAcademy/pulls, make sure all of your commits are present, and then click the "Ready for review" button:

GitHub website screenshot of a draft pull request that's ready for review.



Contributing instructions #2

Draft noahmclean wants to merge 3 commits into `EARTHTIME:main` from `noahmclean:contributing-instructions`

noahmclean commented 19 hours ago

Instructions for contributing content to Mass Spec Academy.

noahmclean added 3 commits 3 days ago

`start VS Code preview, revise branching`	`98dd267`
`GItHub Desktop commit instructions`	`f420062`
`Contributing: Add pull request screenshots`	`1fc3542`

noahmclean marked this pull request as draft 1 minute ago

This branch has not been deployed
No deployments

No conflicts with base branch
Merging can be performed automatically.

This pull request is still a work in progress
Draft pull requests cannot be merged.

You can also merge this with the command line. View command line instructions.

Reviewers: No reviews

Assignees: No one—assign yourself

Labels: None yet

Projects: None yet

Milestone: No milestone

Development: Successfully merging this pull request may close these issues. None yet

You're receiving notifications because you're watching this repository.

Once your branch is merged, you can check https://massspec.academy/ to see it live – new content should appear in about a minute.

A.4.1 Workflow:

The contribution process now looks like:

1. Start another branch with a new name for your new task in GitHub Desktop,
2. create some new content in VS Code,
3. commit the content on GitHub Desktop with a descriptive commit message,
4. create a draft pull request using GitHub Desktop and GitHub.com,
5. keep writing and committing as you go, then

6. when you're done, indicate on GitHub.com your pull request is ready to review.

A.4.2 Authoring

For Quarto syntax and formatting, like headings, figures, equations, and more, check out the Authoring Guide on the https://quarto.org/ website.

A.4.3 Code additions

The current conda environment includes Python 3.13 and Jupyter notebook requirements along with numpy, pandas, matplotlib, seaborn, and bokeh. If you need additional requirements for the code you wish to include in Mass Spec Academy, then you can add them to the environment, then export them to the environment.yml file.

B Citing Mass Spec Academy

Mass Spec Academy is maintained by the project maintainers in collaboration with a group of editors and section authors. The materials that make up MSA are maintained in a Github repository that is part of the EARTHTIME organization. Updates are periodically pushed to the website and assigned a version number. The current version is 0.1.

Citations in peer-reviewed published work should refer to the version number using the format below, and should include the full author list. Dynamic citations may refer to individual sections but we recommend that they also include the version number and access date. You can access past versions and changelogs below.

B.1 How to cite the web version in static work

If your work will be peer-reviewed and published online or in print as either a static resources (like a journal article) or with a version number, use the citation format below to refer to the specific version of the website that you accessed. Refer in text to the specific section referenced if necessary.

Cox, S. E., Mclean, N. M., Arkula, C., Cruz-Uribe, A. M., Ickert, R, B., Lloyd, M. K., Panahi, F., Piasecki, A. M., Runyon, M. L., Souders, A. K., Tremblay, M. M. Mass Spec Academy, v. 0.1, https://massspec.academy/versions/web/v0_1.

B.2 How to cite the pdf or printed version in static work

Mass Spec Academy will be availabled as a printed and static pdf resource starting with version 1.0.

B.3 How to cite sections using a hyperlink in web and dynamic resources

If your work refers to a section of Mass Spec Academy using a hyperlink and does not require a traceable reference, you may directly link to https://massspec.academy or to specific sections of the web resource. However, we recommend including information about the version and date of access to avoid confusion if MSA is updated. You may also use the versions list below to access static versions for direct hyperlinking.

B.3.1 Versions

Static versions will be periodically compiled and listed here along with a changelog. The links below refer to older versions of the live resource that will not be changed, and the corresponding files are also available in version-specific branches on Github.