

## PROPOSED RESEARCH

### 1 INTELLECTUAL MERIT

Many biologists believe that Earth will experience a 6<sup>th</sup> mass extinction if we do not rapidly alleviate threats to biodiversity (e.g., 1-5). However, which conservation efforts will be most effective remain difficult to determine, given the unprecedented rate of environmental change (e.g., 6-9). Understanding how the Earth system responded to past extreme forcing events informs our understanding of how it will respond in the future. Like current climate change, the Cretaceous-Paleogene (K-Pg) mass extinction (66 Ma) had a geologically abrupt onset (e.g., 10-13). Further, as the most recent and well-documented mass extinction, the K-Pg boundary provides a unique opportunity to understand the spatial and temporal patterns of extreme biotic change. **Here, we propose Earth system model development and simulations in combination with new soot, paleotemperature, and organic geochemical analyses to determine the mechanisms responsible for mass extinction and recovery across the K-Pg boundary.**

The majority of geoscientists agree that the Chicxulub impact was primarily, if not solely, responsible for the K-Pg mass extinction (11, 14, 15). Nevertheless, debate continues about what impact-driven processes ultimately caused the extinction. A main reason for this continuing dispute comes from our poor understanding of Earth system responses to extreme perturbations. Ambiguity concerning forcings and feedbacks has allowed for the perpetuation of many extinction hypotheses, including rapid cooling and cessation of photosynthesis from aerosol injections (e.g., 16-22), acidification from gas release (e.g., 14, 23-26), burning from a thermal pulse (e.g., 27-30), ultraviolet radiation from ozone destruction (e.g., (21, 31), and warming from greenhouse gas emissions (e.g., 32-34). Most likely, the kill mechanism was a combination of processes that acted at varying timescales, and with different forcings being largely responsible for extinctions among distinct ecosystems, for individual taxa within a single ecosystem, and between similar ecosystems located at varying distances from the Chicxulub impact (e.g., 13, 20, 35, 36).

Earth system models are a powerful tool for quantifying the consequences of different extinction hypotheses (37, 38). Previous modeling efforts have proven invaluable to furthering our understanding of the devastating consequences from the Chicxulub impact (14, 15, 17, 21, 22, 29, 32, 39-46), but all have limitations in either boundary conditions, forcings, or model complexity. To date, there has yet to be a complete representation of the forcings from the Chicxulub impact using an Earth system model.

Accurate simulation of the Chicxulub impact is a major challenge because it requires adapting an Earth system model for both deep time climate and extreme perturbations. However, the current generation of Earth system models have the capability to go beyond previous efforts (e.g., 21, 22, 45, 47, 48). For the first time, new model components allow us to fully test hypotheses surrounding the K-Pg extinction. Here, we propose adapting an Earth system model, which includes an explicit aerosol resolving scheme and an ocean biogeochemistry-ecosystem module with integrated carbon isotopes, to simulate many of the physical, chemical, and biological responses across the K-Pg boundary. These simulations will allow for direct comparison with proposed and existing sedimentological, paleontological, geochemical, and climatological records, providing unprecedented insight into the mechanisms responsible for the K-Pg extinction.

Emissions from the Chicxulub impact are difficult to constrain without proxy reconstructions to verify the magnitude and nature of environmental responses. The challenge in performing such empirical tests of predicted climatic and biological change is finding archives of paleoecological and paleoenvironmental relevance that have sufficient fidelity and temporal resolution to be useful in discriminating among alternative hypotheses. The combination of geologically abrupt forcings (e.g., 43, 49), extinction of many calcareous microfossils (e.g., 50-53), and poor preservation and reworking of microfossils that are present (e.g., 54-57) are all complicating factors affecting different aspects of the K-Pg record in disparate ways. For example, records of the synchronicity and rate of biological changes are relatively well resolved (e.g., 12, 13, 25, 50, 51, 54-56, 58-64). On the other hand, details about the temperature history across the boundary on short time scales remain less established. Using a variety of proxies in terrestrial and marine sections, some studies have reported temperature patterns consistent with prominent predictions of global changes from Chicxulub impact emissions, including impact winter and subsequent greenhouse warming (33, 34, 49, 65, 66), whereas others have reported patterns variously explained by regional oceanographic responses to the Chicxulub impact (e.g., 15, 67-70). Uncertainty regarding temperature response across the K-Pg boundary, limitations in existing empirical data on soot and polycyclic aromatic hydrocarbon (PAH) concentration, and limited biomarker evidence of ecosystem changes all compromise efforts to discriminate

among modeled forcings; these are all explicit targets of the model-data integration proposed here.

Our broad-scale interdisciplinary research (**Figure 1**) couples proxy and modeling approaches to concurrently examine several hypotheses for K-Pg extinction. This includes 1) the integration of sedimentary soot (%soot C, and  $\delta^{13}\text{C}$  soot) and forest fire biomarker (PAHs) records with explicit aerosol dispersal modeling, 2) the evaluation of high resolution paleotemperature records (using both resistant phase  $\delta^{18}\text{O}$  of fish debris and the biomarker-based  $\text{TEX}_{86}$  paleothermometer) with  $\text{CO}_2$  pulse simulations that include prognostic carbon cycling, and 3) the interpretation of planktonic ecology and marine productivity reconstructions based on biomarker ratios and concentrations with outputs from an integrated ocean biogeochemistry-ecosystem model. All new proxy reconstructions will provide sufficient temporal resolution to compare directly with model experiments. This proxy-model comparison will allow us to capture the abrupt environmental changes that may have driven the K-Pg impact winter, as well as the climate change in the millennia around the boundary. Our modeling experiments will test if perturbations large enough to match the biological, sedimentological, and geochemical record are possible without invoking a large increase in greenhouse gases at the K-Pg boundary. For example, finding  $\delta^{18}\text{O}$  for 5°C warming in the first  $10^5$  years after the boundary correlated with evaluated soot inputs at many sites would favor models that include a significant increase in  $\text{CO}_2$  and widespread fires. Alternatively, if there is no evidence of post-boundary warming as predicted by Hull et al. (15), model scenarios will be favored that do not invoke a large increase in greenhouse gases at the K-Pg boundary but still create perturbations large enough to force extinctions, disturb the carbon cycle, and match the distribution of soot and biomarkers.

In short, our team will use a combination of state-of-the-art Earth system model simulations with detailed soot analyses, and high temporal resolution paleotemperature records and biogeochemical reconstructions to provide a detailed picture of the likely environmental responses to the Chicxulub impact. Ultimately, this project will help us answer a fundamental research question about Earth's history:

**Q: How did the earth system respond in the months to millennia after the Chicxulub impact?**

Specifically, our proposed research activities will allow us to test the following hypotheses:

**H1: The Chicxulub impact caused widespread fires and soot emission, which was a primary contributor to the impact winter.**

**H2:  $\text{CO}_2$  emission from the impact site and widespread fires resulted in several degrees of warming in the millennia after the Chicxulub impact.**

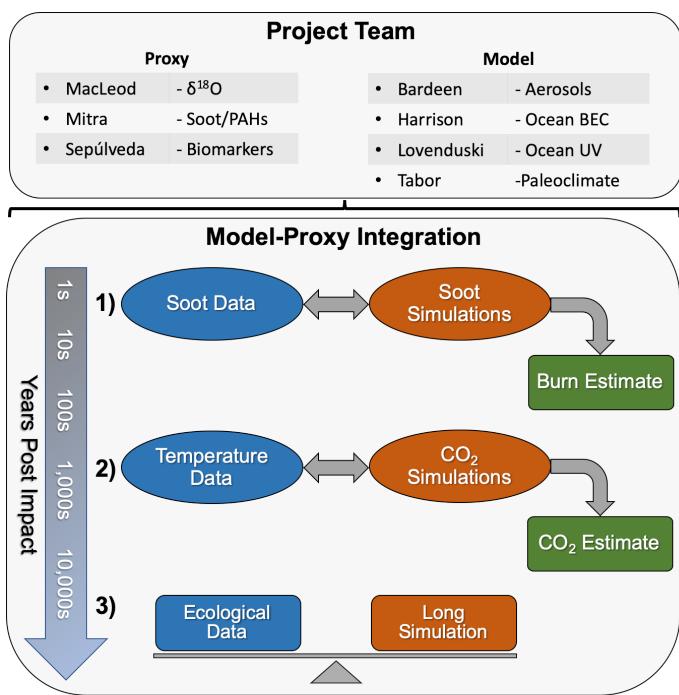
**H3:  $\text{CO}_2$  and sulfur emission from the impact drove ocean acidification, which delayed the marine recovery and contributed to the loss of the  $\delta^{13}\text{C}$  gradient.**

**H4: Ozone destruction from Chicxulub impact emissions exacerbated the extinction and delayed the recovery by increasing surface UV exposure.**

## 2 SCIENTIFIC BACKGROUND

### 2.1 Chicxulub Asteroid Impact

The K-Pg boundary is dated to ~66 Ma (71-73) and coincides with an abrupt, global decrease in biodiversity. Across the boundary, 40% of genera were lost and >75% of all species went extinct (4, 74, 75). Despite global disruption, extinction magnitudes and recovery timelines vary by biological class and region (e.g., (13, 20, 35, 36, 62, 76). In 1980, Alvarez et al. hypothesized that an asteroid impact was responsible for the K-Pg mass extinction based in large part on observations of anomalously high concentrations of iridium at the boundary in several widely separated sites. More than a decade later, the 180-200 km impact crater was identified in the Yucatan Peninsula, near the village of Chicxulub (77). The impact left a unique geophysical scar on the landscape (e.g., 78). Paleogeographic reconstructions of the latest Maastrichtian suggest the asteroid landed in a ~650 m deep coastal sea (79). This once-in-a-100-million-years impact released a formidable amount of energy, likely in the range of  $10^8$  Mt of TNT (19, 38, 80). Although not a consensus opinion, the most widely accepted explanation for the K-Pg extinction is currently the Chicxulub impact and subsequent ecological cascades (e.g., 11, 36).



**Figure 1.** Model-proxy integration. Our project will -  
 1) Constrain fire emissions with soot records and short soot deposition simulations  
 2) Constrain CO<sub>2</sub> emissions with temperature records and 1-kyr CO<sub>2</sub> sensitivity simulations  
 3) Compare detailed ecological records with 50-kyr ocean biogeochemistry simulation

years, lowering surface temperatures and hampering photosynthetic activity (18, 20-22, 38, 39, 43, 45, 102). Likewise, nanoparticles and submicron clastics emitted from the collision likely also blocked sunlight from reaching the surface for months after the impact (41, 103, 104).

The Chicxulub impact produced many gases known to affect climate. Given the expected composition of the impactor and target material (105-108), the collision should have led to significant emissions of sulfur, carbon, water vapor, chlorine, bromine, iodine, and nitrogen (e.g., 23, 38, 42, 43, 86, 109-112). Sulfur gas came mainly from the target material. Total emissions were possibly in excess of 1000-times the amount emitted by the 1991 Pinatubo eruptions and subsequent sulfate aerosol formation should have caused global cooling and acid rain (14, 22, 42, 43, 46, 105, 110, 112-114). On the other hand, carbon (as CO<sub>2</sub>) and water vapor, resulting from fires and vaporized target material, could have led to warming, especially after other aerosols and gases settled out of the atmosphere (32, 38, 42, 110, 115). CO<sub>2</sub> in particular could have warmed the climate for many millennia after the impact (e.g. 33, 116) although a recent study argues against a post-impact greenhouse interval (15). Finally, the impactor, sea water, and fires together likely emitted large quantities of halogen gases (31, 38, 43). Post-impact concentrations of stratospheric chlorine, bromine, iodine, and NO<sub>x</sub> could have been elevated several hundred to thousand times above background levels, causing ozone destruction and leading to a spike in surface ultraviolet radiation after the removal of other radiation blocking aerosols.

There are a number of challenges to constraining changes across the K-Pg with observational data. Many effects occurred on timescale far below the temporal resolution of the geologic record at most sites. For example, reduction in sunlight due to emissions from the impact should only have lasted for several months to a decade (19, 21, 22, 43, 86, 100), whereas typical sedimentation rates in well studied sites are less than a cm/kyr. Physical reworking, bioturbation, and chemical remobilization introduce additional complications (82). Where the anomalous signals are orders of magnitude above background levels, instances like the iridium spike, it may be possible to discriminate among instantaneous, gradual, and repeated inputs of anomalous material with sediment mixing models (e.g., 36). Such approaches do not work well for paleotemperature records but might be useful interpreting new measurements of soot

The Chicxulub impact caused tsunamis reaching more than 300 km inland (81-84), earthquakes in excess of magnitude 11 (43), and collapse of the Yucatan carbonate shelf (85), all of which would have decimated local biology. Simultaneously, a variety of particulates and vapor composed of material from the impactor and target site were ejected into the atmosphere (41-43, 86). Much of this debris subsequently rained down to Earth, as recorded in sediment records from around the globe (11, 51, 82, 83, 87, 88). A pulse of thermal radiation associated with frictional heating from the reentry of particles may have resulted in widespread fires (28, 29, 38, 89), consistent with the presence of a K-Pg soot layer containing aciniform (grapelike) structured-carbon and pyrogenic PAHs interpreted as evidence of a massive, quick deposition of burned material (90-95). While debate continues about the source of this soot (30, 45, 80, 96-101), the data in these studies largely suggest that elevated amounts of soot (0.02 g cm<sup>-2</sup>) rapidly entered the atmosphere (91). If the soot injection reached the stratosphere, it would have significantly reduced the amount of sunlight reaching Earth's surface for many

abundance or PAHs. On the other hand, exceptionally high resolution temperature records could be generated in sections where sedimentation rate is relatively high, chronostratigraphy is well documented, and sedimentary structures, such as laminated (as at Stevns Klint, (117) or undisturbed normal grading (as at Demerara Rise, (51, 118), are present and argue for minimal bioturbation. Data from such sites can be used to test if short-term climate and biochemical signals are present. Diagenesis also can compromise the record and carbonates are relatively susceptible to alteration. Thus, targeting exceptionally diagenetically resistant phases (e.g., bioapatite) and lipid biomarkers increase the rigor of the study.

## 2.2 Model Simulations

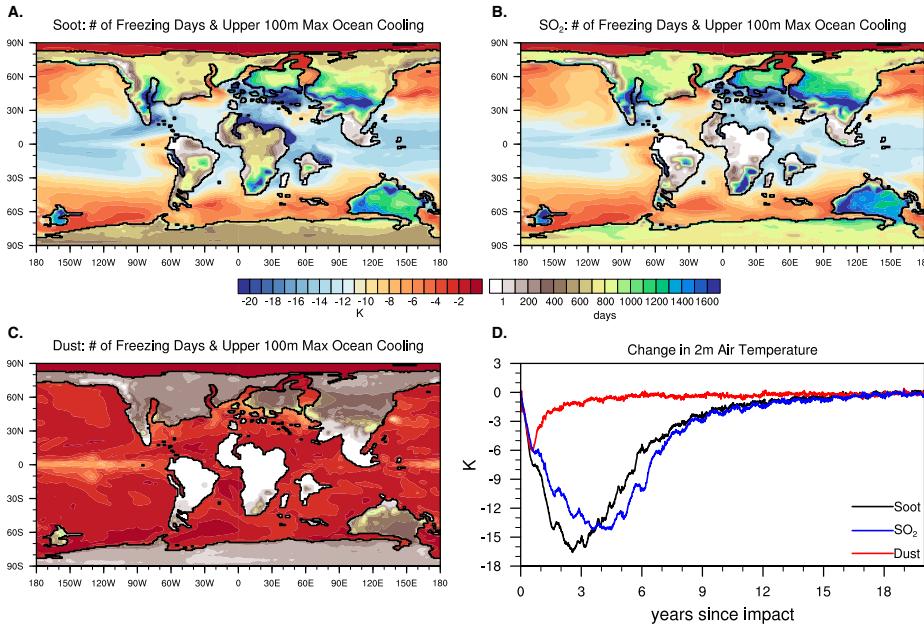
Models are valuable tools for understanding the climate responses to emissions from the Chicxulub impact (37). However, the combination of a mean-state far removed from present-day and extreme forcings have proven difficult to simulate. Consequently, previous K-Pg modeling experiments have been limited in number and scope.

Emissions from the Chicxulub impact are multifaceted. Previous efforts simulate certain aspects of these forcings with models of varying complexity. Early studies using radiative transfer and 1-D models demonstrate that dust emissions from the Chicxulub impact can reduce light to levels below those required for photosynthesis (17, 39, 43). Likewise, simple simulations suggest that SO<sub>2</sub> emissions are able to reduce surface sunlight for one or more decades (19, 42, 110). Using present-day geography, Covey et al. (41) conducted the first global climate simulations of a perturbation from the Chicxulub impact. Like others, they simulate a reduction in sunlight from dust emissions, which leads to rapid decreases in temperature. In addition, the greater complexity of their simulation illustrates the heterogeneity of the temperature response and a reduction in precipitation from a Chicxulub-size dust emission.

In the past few years, there has been a surge in the number of Chicxulub impact modeling experiments. Earth system modeling studies with explicit aerosol transport show that soot can have profound impacts on the climate system, even under low-end emission estimates, by reducing sunlight at the surface (21, 22, 45). Bardeen et al. (21) also simulated the effects of water vapor and CO<sub>2</sub> emissions but found them to be of secondary importance to the climate response in the decades after impact. Another recent Earth system modeling study, using Maastrichtian boundary conditions and a simplified atmosphere, explored SO<sub>2</sub> and CO<sub>2</sub> emissions from the impact (46). In that study, SO<sub>2</sub> emissions result in rapid surface cooling followed by warming from the CO<sub>2</sub> increase. Joshi et al. (32) find potential for long-term warming due to stratospheric water vapor injected at the time of impact. Recently, Henehan et al. (14) used the intermediate complexity model, cGENIE, to explore the reduction in marine primary productivity necessary to reduce the δ<sup>13</sup>C gradient as found in observations (e.g., 119). In agreement with several previous proxy works, they find that a complete loss of primary productivity is not necessary to replicate the records. Although the limited complexity of their model forced them to prescribe the initial reduction in primary productivity, their work highlights the value of long simulation with ocean biogeochemistry for interpreting the complexity of K-Pg proxies. Finally, using a complex model with explicit aerosol resolving scheme, Tabor et al. (22) looked at individual asteroid emissions of dust, SO<sub>2</sub>, and soot and found that soot would be the primary driver of impact winter if the asteroid impact led to widespread fires (**Figure 2**). While simulations of the Chicxulub impact are advancing, all modeling efforts to date provide incomplete representations of the forcings and responses. Below, we outline a modeling framework that will allow us for the first time to systematically simulate many of the previously overlooked Earth system responses to the Chicxulub impact.

## 2.3 Temperature Estimates

Temperature change across the K-Pg boundary has been the focus of a number of recent papers with direct implications for K-Pg forcing. Hull et al. (15) presented a compilation of paleotemperature data and convincingly argued that the long-term record does not match expected temperature patterns for volcanic forcing of the K-Pg boundary event. The compilation is an excellent product, similar to what we proposed assembling in earlier drafts of this proposal. We are happy both that the task is complete and that the product demonstrates the power of temperature records to discriminate between alternative hypotheses.



**Figure 2.** Temperature response to impact aerosols. Maximum cooling in the upper 100m of the ocean and number of days with below freezing temperatures beyond climatology after emission of (A) soot, (B) SO<sub>2</sub>, and (C) dust. (D) Change in global average 2m temperature after aerosol emission relative to climatology. Results highlight the ability of the model to distinguish among the effects of different impact winter aerosols. Modified from Tabor et al. (2020).

Kef K-Pg GSSP (33) and their own bulk carbonate  $\delta^{18}\text{O}$  measurements at IODP Site U1403 in the NW Atlantic suggest 5°C warming, but the paper considered those measurements anomalous. Other reports of significant post-impact warming do exist, though. TEX<sub>86</sub> evidence from New Zealand suggests a 3–5°C increase (66), while records data from New Jersey suggests 2–3°C increase (65) at the boundary. Leaf physiognomy in the Denver Basin suggest 5°C temperature increase within the 1<sup>st</sup> 60,000 years of the Paleogene correlated with a dramatic increase in the size of contemporary mammals (34). Finally, in a pilot study, we found a large decrease in  $\delta^{18}\text{O}$  values suggestive of 5–7°C warming among mixed assemblages of small (<125  $\mu\text{m}$ , >63  $\mu\text{m}$ ) planktonic foraminifera at Demerara Rise within the 1<sup>st</sup> 50,000 years of the Paleogene (**Figure 3**). In short, despite the rigor of the Hull et al. (15) compilation, enough recent studies using a variety of techniques in a variety of settings from widespread localities have found evidence of warming to consider it a viable alternative hypothesis. Documenting  $\delta^{18}\text{O}$  values in fish debris at Stevns Klint, Denmark with an emphasis on samples from the 35 cm thick phosphate-rich boundary clay representing the first 10,000 years of the Paleogene (122) would be means to test for post-impact warming using a diagenetically resistant phase from an expanded and well-studied section with sedimentary structures indicating of lack of bioturbation and depositional depths of a few hundred meters limiting the range over which the fish analyzed might have lived (33).

On shorter times scales, provocative hints for the occurrence of an impact winter following the K-Pg boundary has been provided by TEX<sub>86</sub>-based temperature estimates that use the archaeal cell membrane lipids glycerol dialkyl glycerol tetraethers (GDGTs) (123). In sections from both Texas and New Jersey, TEX<sub>86</sub> shows low values in some samples above the boundary relative to samples higher and lower in the sections, suggesting a cooling of 5–8°C in less than 100 years after the Chicxulub impact (49, 65). These studies have not been easy to replicate. The biomolecules needed have not yet been isolated from outcrop samples from the EI Kef locality (68) or the Stevns Klint locality targeted for detailed study here (122). However, well preserved biomarkers are present at Stevns Klint (122) and recently recovered drill cores from EI Kef (124) open the possibility that extracting larger and fresher samples will yield measurable abundances of GDGTs.

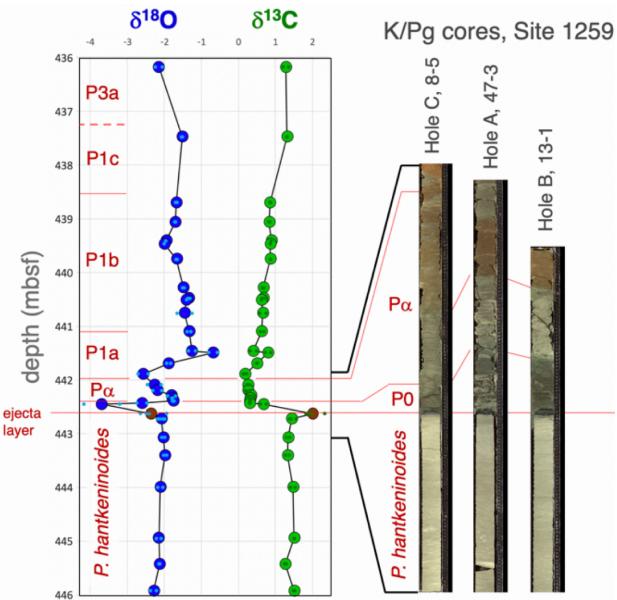
## 2.4 Burn Estimates

In addition to testing impact vs. volcanic forcing, Hull et al. (15) argued that there was no evidence of post-impact warming, consistent with recent studies predicting only modest generation of CO<sub>2</sub> (~50 ppm) due to volatilization of target rocks (112, 120, 121). Implicitly, lack of post-impact warming also argues against substantial biomass burning, which might have introduced >300 ppm CO<sub>2</sub> (21, 38). Hull et al. (15) noted that both  $\delta^{18}\text{O}$  analyses of fish debris from the EI

The pioneering studies of the K-Pg boundary clays at sites such as Woodside Creek, Flaxbourne River, and Chancet Rocks, NZ, Stevns Klint, DK, Caravaca, ES, Gubbio, IT, all established that concentrations of soot and PAHs were present at and above the K-Pg boundary at concentrations indicative of widespread wildfires (91-94). Indeed, the ratio of soot to total sedimentary organic carbon in the NZ boundary clays was ~70% (94). The technique for isolation of soot is based on the kinetics of the reduction reaction of an acidic solution of  $\text{Cr}_2\text{O}_7^{2-}$  in conjunction with that solution's simultaneous oxidation of reduced organic matter. The acid- $\text{Cr}_2\text{O}_7^{2-}$  oxidizes labile and refractory carbon ranging from fresh biomass to kerogen and even labile pyrogenic carbon, depending on the duration of oxidation time (125). It is also assumed that each fraction of total organic carbon present in the sample responds differently to the excess oxidant. The oxidation of carbon in the residue during the etching procedure is then modeled as a first-order exponential loss process, with a "fast" rate constant corresponding to labile non-pyrolytic carbon, intermediate rate constants corresponding to kerogens, and a "slow" rate constant corresponding to truly pyrolytic carbon (e.g., elemental carbon). The mass fraction of soot is then quantified from this elemental carbon residue using planimetric analysis of a scanning electron microscopy (SEM) image. Specifically, soot is distinguished by its "acinariform" morphology (95, 125). Although this technique has been applied to K-Pg and modern sediments (for a review see (126), the toxicity of the reagents, and the lengthy duration and robust nature of the etching in the face of limited sample amounts, present challenges. In contrast, the CTO-375 technique has been the technique most widely applied to soils and sediments to isolate pyrolytic carbon (127), specifically soot (128). This method consists of acidification of a sedimentary sample with 1N HCl and then a thermal oxidation of OC in the presence of excess air, slowly ramped from 23 to 375 °C (127). The residual sedimentary carbon is then quantified by CHN elemental analysis. This latter method has been successfully used to isolate soot carbon in lake sediments associated with the Younger Dryas Impact Hypothesis (129). Given the potential importance of soot in the K-Pg extinction (21, 22, 45) and the continued debate about the extent of fires (e.g., 30, 98), additional soot measurements are critical for understanding the causes of climate change across the boundary.

## 2.5 Biomarkers as Ecological Markers

The fossil record of calcareous microfossils provides only a partial view of marine ecosystems that is restricted to organisms with a hard fossil record. Thus, there is a need for more comprehensive approaches to study the response of marine ecosystems and biogeochemical cycles to transient and long-term environmental perturbations across the K-Pg boundary. Biomarker-based records have the potential of unraveling the role of eukaryotic and prokaryotic picoplankton such as naked algae, archaea, and nitrogen-fixing cyanobacteria during periods of extreme environmental change and ecological turnovers (122, 130-135). To date, the response of non-calcifying plankton, and its role in controlling marine productivity and ocean biogeochemistry following the collapse of calcifying plankton across the K-Pg boundary, remains



**Figure 3.** Mixed planktic foraminifera (> 63  $\mu\text{m}$ , < 125  $\mu\text{m}$ ) oxygen and carbon ratios from ODP Hole 1259C showing the preservation of the well documented rapid decrease and gradual recovery of  $\delta^{13}\text{C}$  values in the planktic realm, evidence of modest warming at 442 mbsf and suggestion of more dramatic warming immediately above the K-Pg boundary (442.5 mbsf). Note drilling disturbance has compromised recovery of the earliest Danian claystone in Hole A whereas is more completely recovered in Holes B and C. The boundary interval was also recovered at Sites 1258 and 1260 so opportunity to test and refine results exists. However, preservation is only very good to moderate in these samples. Small circles represent individual analyses with large circles representing average values for a given samples; brown circles denote values from specimens within the ejecta layer.

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largely unexplored. Lipid biomarker data from neritic environments such as the classic Fiskeler section in Denmark indicates a rapid (centennial to millennial time-scale) resurgence of primary productivity driven by non-calcifying phytoplankton (122). However, similar studies are limited both in number and temporal resolution, which has prevented a more holistic reconstruction of marine ecosystems across this mass extinction event, especially at high temporal resolution. We propose to use fossilized lipid biomarkers to study the structure of planktonic assemblages in response to the K-Pg

stressors. This includes the analysis of aliphatic and aromatic hydrocarbons (n-alkanes, isoprenoids, steranes and hopanes) as well as functionalized lipids (e.g., archaeal tetraethers). In particular, we expect to trace the relative contribution of different groups of eukaryotic and prokaryotic plankton (e.g., 122, 135) at elevated temporal resolution (centennial to millennial) across the K-Pg. Furthermore, we plan to use changes in the absolute concentration (and accumulation rate) of diverse algal biomarkers as indicators of marine productivity and carbon export to the sea floor. Additionally, we will calculate biomarker ratios to infer changes in ocean redox conditions across the K-Pg boundary. This includes the homohopane Index (HHI; 133, 136) as an indicator of changes in bottom water oxygen levels, the 3-methyl hopane index (3MHI) as an indicator of methanotrophic bacterial biomass export (137), the gammacerane index (GI; e.g., 138) as an indicator of water column stratification, and the green sulfur bacterial carotenoids isorenieratane and chlorobactane (139) as indicators of photic zone euxinia (140). Preliminary biomarker results from one of the 5 holes from the El Kef Coring Project (**Figure 4**) demonstrates that these samples exhibit a superior degree of preservation and thermal alteration (124) compared to Stevns Klint (122), which allows for the reconstruction of high-resolution records of ecological and environmental changes across the K-Pg boundary and beyond.

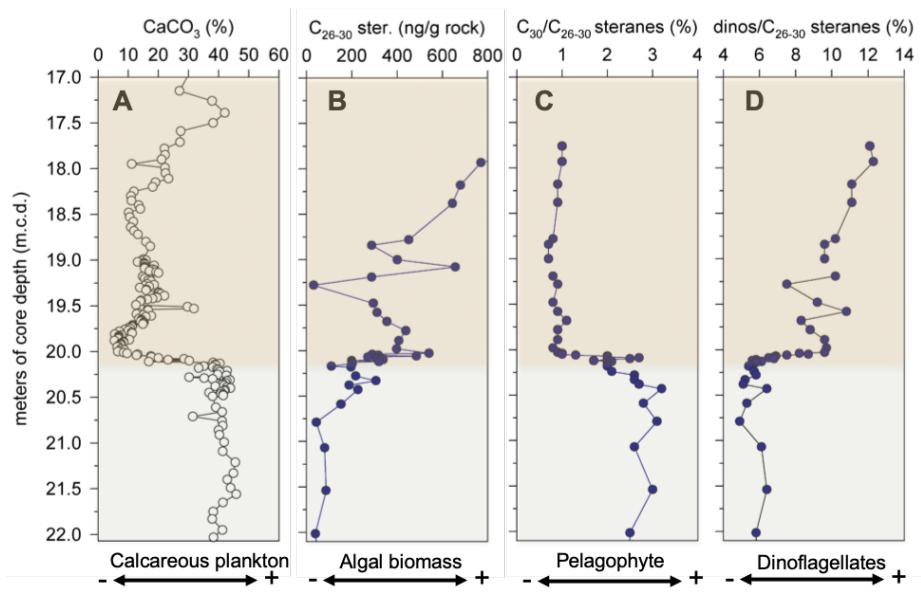
### 3 METHODS

#### 3.1 Earth System Modeling Approach

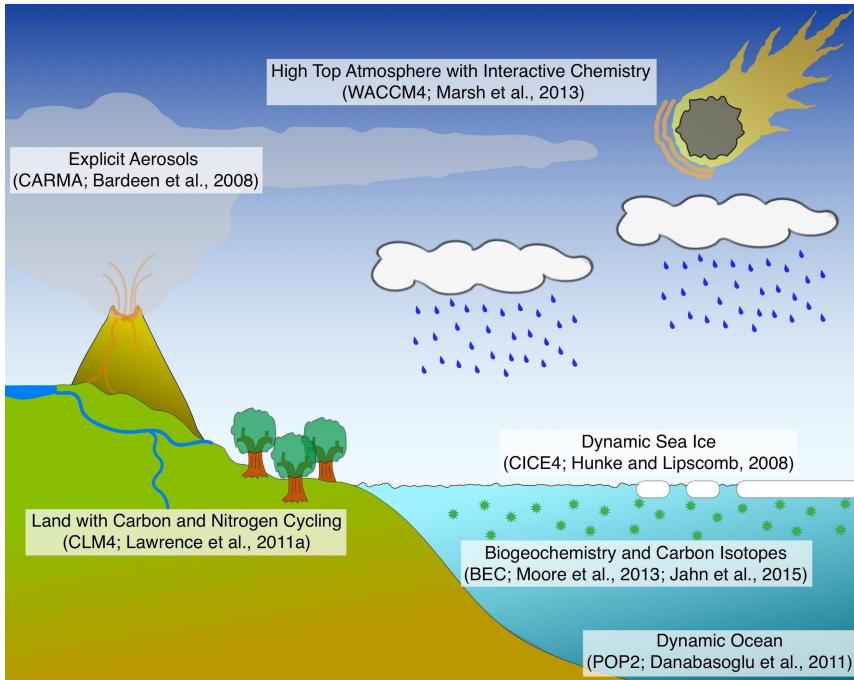
Because of the potential for global disruption from the Chicxulub impact, we require a climate model that simulates all major components of the Earth system (**Figure 5**).

##### 3.1.1 Model Configuration

Here, we propose to use the Community Earth System Model (CESM), maintained by the National Center for Atmospheric Research (NCAR; 141, 142). CESM is a widely employed, state-of-the-art Earth system



**Figure 4.** Preliminary biomarker data from El Kef Coring Project cores 1A-15R, 1A-16R, and 1A-17R: (A) % $\text{CaCO}_3$ ; (B) abundance of total algal steranes ( $\Sigma\text{C}_{26-30}$  steranes in ng/g rock) indicative of bulk algal biomass; (C) relative contribution of C30 steranes (Pelagophyte) to the total pool of algal steranes ( $[\text{C}30/\text{C}_{26-30} \text{ steranes}] \times 100$ ); (D) relative contribution of dinosteranes (dinoflagellates) to the total pool of algal steranes ( $[\text{dinosteranes}/(\text{dinosteranes} + \text{C}_{26-30} \text{ steranes})] \times 100$ ). The K/Pg boundary, shown at ~21 m.c.d. is defined by the transition from nannoplankton Zones 0 to 1. Background colors indicate late Cretaceous (light green) and early Danian (light orange). The results demonstrate that high-resolution records of ecological and environmental conditions across the K-Pg boundary can be constructed using cores from the El Kef Coring Project.



**Figure 5.** Diagram of the proposed Earth system model components. All model components are fully coupled and have been tested in Cretaceous and large perturbation scenarios.

Therefore, we will utilize it for simulation spin-up and long-term post-K-Pg boundary integrations. Depending on the experiment, we will run CAM4 at either high resolution ( $1.9^\circ \times 2.5^\circ$ ) or low resolution (T31;  $\sim 3.75^\circ \times 3.75^\circ$ ) resolution. The low-resolution configuration is considerably less expensive to run yet captures large-scale climate features well (149). The low computational cost of this setup makes it ideal for long-term paleoclimate simulations that we can directly compare with proxy records.

Although CAM4 simulates tropospheric climate well, it cannot capture the middle and upper atmosphere responses to aerosol perturbations associated with asteroid impacts and large volcanic events. For simulations of the Chicxulub impact, we will utilize WACCM4, which is a high-top atmosphere configuration that reaches the thermosphere, at high resolution ( $1.9^\circ \times 2.5^\circ$ ) with interactive chemistry. In WACCM4, we will implement the Community Aerosol and Radiation Model for Atmospheres (CARMA) for explicit aerosol calculations (150, 151). CARMA is unique in that it allows the aerosol size distribution to evolve freely, a necessity when simulating large aerosol injections. This model configuration tracks aerosol (i.e., soot) deposition, which we will use to compare with new and existing sedimentary records from the K-Pg (e.g., 83, 94; **Figure 6**). Such comparisons will allow us to determine the extent of fires necessary to produce the observed spatial distribution of soot and pyrogenic PAHs deposition at the K-Pg boundary and help settle the ongoing debate about the intensity and consequences of the impact-driven pulse of thermal radiation (e.g., 101, 103). Tracking the deposition of aerosols will also help determine where the effects of acid rain are most destructive. Moreover, with the recent addition of in-line TUV (152), we can capture the effects of aerosols on photolysis within WACCM4 to accurately simulate the aerosol responses in the upper atmosphere and potential surface UV increase from O<sub>3</sub> destruction (31). Our UV modeling work will integrate well with a NERC grant recently awarded to Dr. Barry Lomax, who will use sporomorph chemistry to track changes in surface UV across the K-Pg boundary (see letter of collaboration). His new records will help us validate our simulated UV responses while our simulations will help him determine the mechanisms responsible for his UV signal.

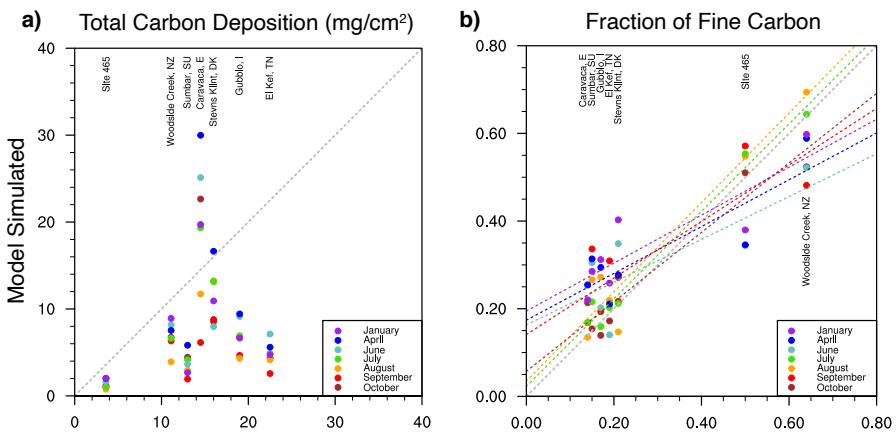
model with the ability to accurately simulate atmosphere, land, ocean, sea-ice, and runoff processes. This model successfully simulates a variety of past climate states, including the Cretaceous, Pliocene, and Last Glacial Maximum (143–146).

We will utilize two versions of the atmosphere model: The Community Atmosphere Model (CAM4; 147) and the Whole Atmosphere Community Climate Model (WACCM4; 148). CAM4 is the standard atmosphere model of CESM, with 26 vertical levels that simulates climate of the troposphere and lower stratosphere. The relatively low number of vertical levels makes CAM4 computationally efficient.

For the ocean component, we will configure the Parallel Ocean Model (POP2; 153) with the Biogeochemical Elemental Cycling (BEC) ocean biogeochemistry model (154, 155), and stable carbon isotope tracking (156) to allow for direct comparison with records of chemical and biological response across the K-Pg boundary. Like the atmosphere, we will run POP2 at either high resolution (nominal 1°) or low resolution (nominal 3°), depending on the experiment. The BEC model calculates the activities of plankton functional types including diatoms, diazotrophs, small phytoplankton, coccolithophores, and zooplankton, which will allow us to simulate the rapid collapse of carbon export (and presumably primary productivity) inferred from the stable isotope composition of planktonic and benthic forams (e.g., 10, 52, 63, 119). In addition, with ocean chemistry, we will be able to test the ocean acidification extinction hypothesis by simulating changes in pH associated with CO<sub>2</sub> increase, cold sea surface temperatures, acid rain (via forced changes in alkalinity (e.g., 15), and changes in ocean mixing (e.g., 14, 25, 114). We will also be able to model the effects of marine hypoxia (57, 157, 158), and the carbon isotope component will be crucial for determining mechanisms responsible for the long-term reduction in the ocean δ<sup>13</sup>C gradient (e.g., 10, 119). Finally, we plan to include the marine plankton sensitivity to UV radiation via modification of the CESM BEC codebase. UV sensitivity will be represented as photoinhibition (a function of the TUV output from the atmospheric component) and carried over to productivity terms via the light limitation function. The sensitivities of plankton to UV will be derived from the literature of laboratory and in situ studies. The plankton response to high doses of UV has not previously been modeled in CESM. The addition of this capability in CESM will allow us to test Hypothesis 4. Further, the development of the codebase to include marine plankton UV sensitivity will aid in future studies of the Earth system response to climate engineering and volcanic eruptions.

We will use the Community Land Model (CLM4; 159) with active carbon and nitrogen cycling for simulating the post K-Pg response on land. Although vegetation types cannot change for a particular grid cell, CLM4 allows plants to grow and die, depending on the environmental conditions. Therefore, we will be able to use this model to determine the spatial patterns of vegetation response to the Chicxulub impact, which we will compare against the fossil records (e.g., 13, 160, 161). We will also use the prognostic carbon cycle in CLM4 to determine the spatial distribution of soot emissions, and estimate terrestrial carbon drawdown and uptake. The horizontal resolution of CLM4 will reflect the atmosphere configurations. The combination of BEC and CLM4 with carbon and nitrogen cycling will capture the dynamic responses of the terrestrial and marine biota to extreme perturbations, which will allow us to directly test the impact winter and pause in photosynthesis extinction hypotheses (17, 18, 102, 162-164). We are also working to update the dynamic vegetation module (DGVM; 165) for use in CESM (145). This addition will allow us to simulate shifts in plant functional types across the K-Pg for more precise comparison with the fossil record.

Previous efforts by the PIs confirm the validity of the modeling approach outlined above. CARMA has been successfully integrated within WACCM4 and stabilized for large aerosol perturbations (21, 22). Further, we have created an equilibrated Maastrichtian simulation, using period appropriate boundary conditions, that compares favorably with sea surface temperature and ocean reconstructions from the Maastrichtian age (145, 166). From this Maastrichtian simulation, we performed K-Pg simulations by adding



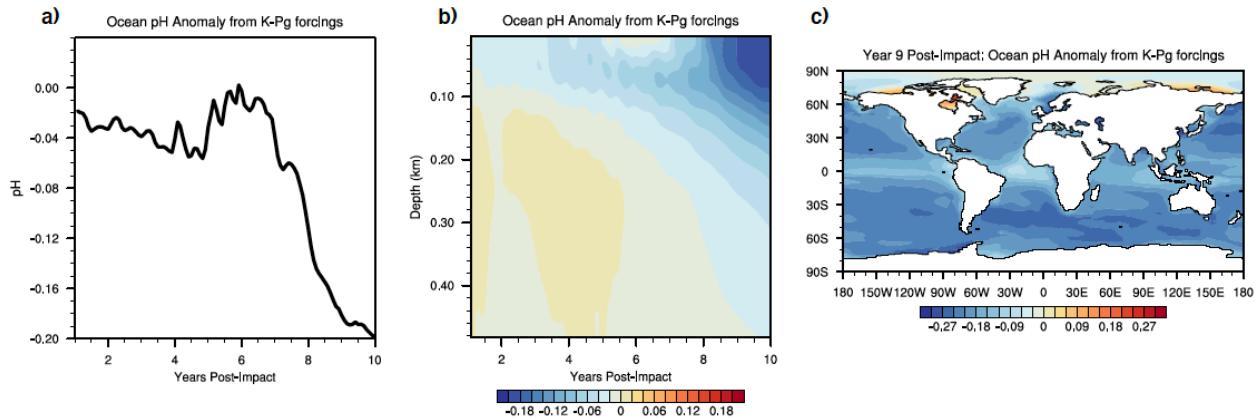
**Figure 6:** A comparison of model simulated and sampled soot deposition at the K-Pg from several sites around the globe (Wolbach et al., 1985; 1988; 1990; 2003). (a) Comparison of soot emission scenarios involving different months of soot emitted at the local tropopause and (b) the relative amount of fine soot contributing to the total soot deposited at the various sample sites. These preliminary results highlight the potential of our simulations to better constrain the amount, location, and timing of soot emission after the K-Pg. The results appear reasonable; however, additional soot analyses and model simulations are necessary to produce robust results.

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individual aerosol emissions of soot,  $\text{SO}_2$ , and dust from the Chicxulub impact. Results show a realistic climate response in the first 20 years after impact, with large differences in response depending on aerosol type (22; **Figure 3**). We have also performed several proof-of-concept simulations for this proposal. First, we compared simulated soot deposition using different seasonality, heights, and durations of emission with existing soot records at the K-Pg (**Figure 6**). Preliminary results suggest general agreement between the model and simulations, especially regarding fine fraction, but additional data collection and simulations are necessary to strengthen these comparisons. Further, we performed a 10-year present-day experiment with the addition of ocean BEC and Chicxulub impact forcings. In our preliminary results, we find a large, complex decrease in surface ocean pH in the years following impact (**Figure 7**). However, we will require the computing time associated with this grant to spin-up ocean BEC for the Maastrichtian and perform long term simulation, which are necessary for comparison with the proxy records.



**Figure 7.** Ocean pH response (anomaly relative to control simulation) to impact aerosols and carbon dioxide emissions from Bardeen et al. (2017). (a) Global change in surface pH, (b) global change in pH of the upper 500 m, and (c) change in surface pH 9 years after impact. This pH signal, which we are still in the process of interpreting, highlights the necessity of complex, fully coupled model simulations when attempting to simulate extreme perturbations such as the K-Pg.

### 3.2 Proxy Reconstructions

Our proposal outlines new analyses at several locations to reconstruct high resolution temperature, soot, and biomarkers across the K-Pg (**Table 1**; **Figure 8**).

#### 3.2.1 New $\delta^{18}\text{O}$ of Fish Debris Temperature Reconstructions

The temperature record across the K-Pg boundary could be critical for testing details of volatile release at the boundary. Specifically, by documenting  $\delta^{18}\text{O}$  values in fish debris at Stevns Klint and  $\delta^{18}\text{O}$  values in species specific separates of foraminifera from Demerara Rise, we propose to test if new data from sections unusually well suited for study of temperatures in the first few hundred to few hundred thousand years of the Paleogene support the finding of the Hull et al. (15) compilation suggesting no post-impact warming or if they provide additional (15, 33, 34, 65, 167; **Figure 3**) evidence for a post-impact greenhouse interval. If we find no evidence of warming, it will suggest the latter studies reflect local signals and will support kill mechanisms and forcings that do not include emission of significant amounts of  $\text{CO}_2$ . Alternatively, if we do find post-boundary warming, our results will strengthen the case for a post-boundary greenhouse interval and put lower limits on possible ranges of  $\text{CO}_2$  likely from wildfires, a possibility to be tested by soot and PAH analyses and model experiments.

Our primary target site for the  $\delta^{18}\text{O}$  of fish debris is the Stevns Klint boundary interval in the Kulstirenden section where the earliest Danian Fish Clay is most expanded (117, 122, 168). The advantages offered by Stevns Klint are numerous. Sedimentation rates were quite high in the basal Danian; the first 35 cm represent ~10 kyrs of deposition and the basal 2 mm record an interval spanning the first decades to century of the Cenozoic (122). In addition, the sediments in the first 15 cm above the boundary are laminated (and laminae continue to be present to 25 cm above the boundary), a sedimentological observation that removes time averaging by bioturbators from the list of complicating factors. The site is estimated to represent water depths of 100 – 150 m (117) limiting the depth range (and temperature range) over which fish might migrate (cf. 33). Organic material of low maturity is present and extractable (122),

and fish debris is unusually abundant in the lower Danian and also present in relatively high abundances in underlying and overlying deposits. Pilot analyses demonstrate feasibility of the proposed study (estimated temperature average 11°C in two Cretaceous samples and 14°C in 3 Danian samples. Finally, Dr. Lars Stemmerik has agreed to collaborate (see letter of collaboration). The value of collaborating with a local scientist with experience on the sections cannot be overstated. Dr. Stemmerik's participation will ensure accurate and efficient field work from the start. We plan cm scale sampling over the upper 25 cm of the Fish Clay, 0.5 cm resolution of the subjacent 8 cm, and as fine as possible in the basal 2 cm as well as cm to decimeter spaced samples in the limestones above and below. We are anticipating analyzing samples from ~200 horizons, as well as replicates (triplicates where possible) and separates of different grain types (e.g. teeth, scales and bone) in selected samples where the abundance of phosphatic microfossils permits such subdivisions.

We also propose analyzing species specific separates of foraminifera from Demerara Rise. The elemental, mineralogical, sedimentological, and paleontological record in the Demerara sites are excellent (e.g., 51, 169, 170). Preservation of the foraminifera is moderate to very good (i.e., not ideal), but the pilot results (**Figure 3**) suggest it is worth investigating. We are targeting up to 4 planktic species and 2 benthic species in each of 50 samples from Sites 1258, 1259, and 1260 for a total of 900 analyses. Dr. Brian Huber will vet foraminiferal identifications (see attached letter of support).

#### Chemical Markers

Site	Temp ( $\delta^{18}\text{O}$ )	Temp (TEX <sub>86</sub> )	Ecology (lipids)	Fires (PAHs)	Fires (soot)
Stevns Klint	This Study	This Study	Sepúlveda et al. 2009	This Study	This Study
El Kef	MacLeod et al. 2018	This Study	Sepúlveda et al. (in prep)	This Study	This Study
Demerara Rise	This Study	No (low organic C)	No (low organic C)	No (low organic C)	This Study
Caravaca	No (diagenesis)	No (thermal maturity)	This Study	This Study	This Study

**Table 1:** All proposed data collection efforts. See text for details.

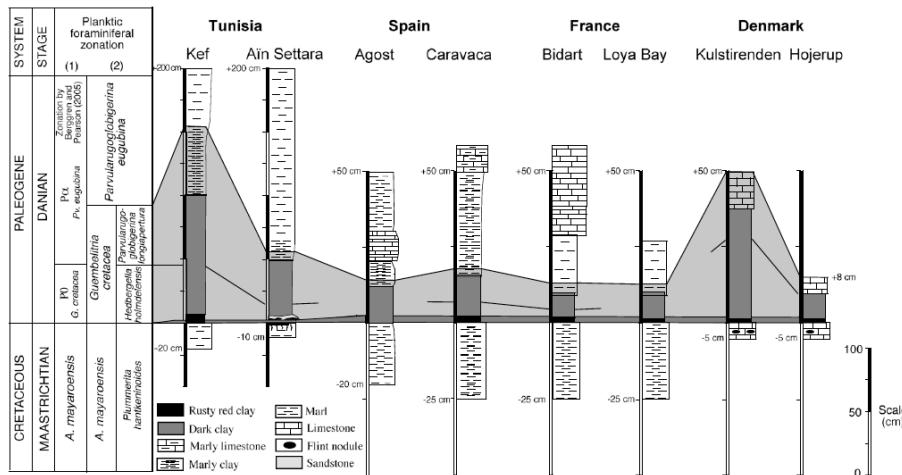
#### 3.2.2 New Soot Reconstructions

New model simulations demonstrate the potency of soot for producing an impact winter (22, 45). Despite hypothetical and observational support for widespread fires after the impact (e.g., 27, 38, 92, 95, 171) uncertainty and skepticism remain (e.g., 98, 101, 103). Further, the techniques used to extract soot have evolved recently (172, 173), making direct comparison between sites difficult. To our knowledge, soot measurements from K-Pg samples have not been performed in at least 17 years and most measurements are significantly older. For all these reasons, we propose to revisit some K-Pg sites analyzed by Wolbach et al. (**Table 1**; Stevns Klint, El Kef, Demerara Rise, and Caravaca). However, rather than soot isolation of the bulk sediment, this team will quantify soot using the CTO-375 technique (127) in different sedimentary size distributions (174). Further, the greater scrutiny of the stratigraphic column, in combination with the reduced sample size required by this technique, will provide us with a better understanding of the timing of soot deposition with respect to the impact. In addition, measuring  $\delta^{13}\text{C}$  of the soot will provide clues about the scale of the burn and amount of atmospheric mixing that occurred before deposition of the soot.

#### 3.2.3 New Biomarker Reconstructions

Organic geochemical studies show that biomarker records provide unparalleled information about planktonic communities that lack hard, calcareous skeletons in addition to environmental conditions such as redox changes (122, 135, 140). This proposal will make use of the published biomarker record from Stevns Klint, Denmark (122), in addition to new expanded records from the El Kef Coring Program (**Figure 4**; Sepúlveda, unpublished data), which includes a not-yet studied expanded Danian section from multiple holes. We note that PI Sepúlveda is a core member of the El Kef Coring Program and has access to these samples. We also plan to analyze new samples from Stevns Klint covering time intervals beyond the existing record by PI Sepúlveda (122). Furthermore, we propose to analyze biomarkers in the well-studied and expanded section of Caravaca, Spain for which multiple bulk and stable isotope geochemical studies have been published (157, 175-178), and for which PI Sepúlveda also has access to samples. Additionally, we plan to study pyrogenic PAHs in all proposed sections where organic carbon is high enough (i.e., Stevens Klint, El Kef, and Caravaca), which we will then compare against soot records to get a more comprehensive reconstruction of paleofires. Whenever possible, we will also analyze GDGTs for TEX<sub>86</sub> in

Stevns Klint and El Kef, which are two sections with good organic matter preservation and a low degree of thermal alteration (122, 124). We highlight that preliminary results from El Kef demonstrate the feasibility of reconstructing ecological and environmental changes across the K-Pg boundary at elevated temporal resolution (>102-103).



**Figure 8.** Biostratigraphy and lithology of several K-Pg boundary sections studied in Sepúlveda et al. (2019). The light gray area with connecting lines indicates the Guembelitria cretacea zone across all sections. Our proposal includes the sections with the most expanded K-Pg boundaries (El Kef, Caravaca, and Kulstirenden).

shallow and deep marine settings worldwide. Moreover, because the K-Pg has been a popular topic of study for many decades and because completeness of individual sections interpretation, there is a large body of literature on the biological, geochemical, and environmental changes at sites representing terrestrial and marine realms with chronostratigraphic control usually explicitly addressed. Our Earth system modeling results will allow for direct comparison with many of the data collected in previous studies. Our primary source for model-proxy comparison will come from the recent K-Pg paleotemperature and carbon isotope compilation by Hull et al. (15). Comparison of previous data analysis efforts with our new simulations will serve three main purposes: 1) to validate that the model is able to accurately capture the environmental responses to emissions from the Chicxulub impact, 2) to constrain better the magnitude, timing, and duration of emissions, and 3) to understand the proxy signals at a mechanistic level. Unfortunately, most of the currently available records that span the K-Pg do not have the temporal resolution necessary for our proposed simulations.

## 4 RESEARCH PLAN

### 4.1 Earth System Model Simulations

We propose a total of 28 K-Pg experiments (**Table 2**). These simulations will require significant computational resources, supported by a combination of facilities at NCAR and the University of Connecticut (UConn). PI Tabor has successfully written several large allocation requests in the past and currently serves on the CHAP review panel. Please see supplemental document of proposed large allocation request for computing on the Cheyenne supercomputer, supported by NSF.

#### 4.1.1 Model Spin-up

As mentioned above, we have an equilibrium Maastrichtian simulation that is stable under extreme aerosol loading. However, we still need to spin-up the ocean BEC model and isotopes with the end-Cretaceous boundary conditions. Previous work by Jahn et al. (156) found BEC and  $^{13}\text{C}$  require ~3,000 years to equilibrate. To reduce computational expense and time, we will use the low-top atmosphere model at high resolution (26 vertical levels on a  $2.5 \times 1.9^\circ$  horizontal grid) in combination with the high-resolution ocean configuration (nominal  $1^\circ$ ) and an asynchronous coupling technique that reduces computational costs by ~50 % (Keith Lindsay, personal communication) for BEC and isotope spin-up. We will also use this technique to spin-up a  $3^\circ$  ocean case for use in our long duration simulations.

### 3.2.4 Data Compilation

The K-Pg extinction is the most recent of the “Big 5” mass extinctions in Earth’s history. Consequently, records from the K-Pg boundary are some of the most temporally and spatially well documented examples of mass extinction with hundreds of sites known (e.g., 11, 15). The boundary including impact ejecta provides an isochronous marker that can be recognized across terrestrial,

From our high resolution equilibrium simulation, we will switch to WACCM4 (66 vertical levels on a 2.5 x 1.9° horizontal grid). The switch from CAM4 to WACCM4 is not a major climate transition because both models use the same underlying physics. However, we will need to spin-up the chemistry in WACCM4. Our tests suggest that chemistry only takes ~15 years to equilibrate (21). To generate a stable pre-perturbation climatology, we plan to run the WACCM4 spin-up simulation for 50 years. This fully-coupled WACCM4 + BEC control simulation will serve as the initial conditions for our subsequent perturbation experiments. The perturbation experiments will maintain the same configuration with the addition of CARMA for explicit aerosol calculations. We will also use forcings from the perturbation experiments in the low-resolution configuration with ocean BEC (atmosphere / land: ~3.75° horizontal grid; ocean / sea ice: ~3° horizontal grid) to produce a 50 kyr simulations that resolves the long-term Earth system responses to Chicxulub impact.

**Model Simulations**

Experiments	Number of Simulations	Duration (years)
<b>Initialization:</b> BEC Spin Up (CAM High Res)	1	3,000
<b>Initialization:</b> BEC Spin Up (CAM Low Res)	1	3,000
<b>Initialization:</b> High-Top Spin Up (WACCM High Res)	1	50
<b>Short:</b> Soot Sensitivities (WACCM High Res)	19	2
<b>Intermediate:</b> All Forcings (WACCM High Res)	1	50
<b>Intermediate:</b> CO <sub>2</sub> Sensitivity (CAM High Res)	4	1,000
<b>Long:</b> All Forcings (CAM Low Res)	1	50,000

**Table 2:** All proposed model simulations using our Earth system model. See text for details.

#### 4.1.2 Emission Estimates

Modeling efforts will be focused on the months to millennia consequences of the Chicxulub impact. We propose several emission scenarios to understand the role of different emissions and their interactions. Unless otherwise noted, our emission sizes and height distributions come from the recent literature synthesis by Toon et al. (38).

- **Soot:** Both our experiments and other modeling works (21, 22, 45; **Figure 2**) suggest that soot could have been a dominant post-impact driver of climatic change by limiting shortwave radiation at the Earth's surface. However, researchers remain uncertain about the extent of fires produced from the reentry of ejecta (e.g., (98, 101). We will refine the amount, size distribution, duration, and timing of soot emission using a series of model sensitivity tests compared against results from our new soot analyses (see 4.1.3 Soot Sensitivity Tests). In all cases, we will emit soot from all land-surfaces, scaled by simulated local vegetation density.
- **Nano-particles:** Coexisting with the global iridium layer are iron-rich particles 15-25 nm in diameter (e.g., 88, 179). Because nano-particles from the impact are dense and tend to forward scatter light (22, 38), we anticipate only a short-lived blocking of sunlight and cooling. Therefore, despite uncertainties in the total amount of nano-particles emitted, the uncertainties in climate response are relatively small. We propose emitting 2,000,000 Tg of nano-particles based on recent estimates (38).
- **Water:** The shallow sea impact site (79) would have resulted in the emission of an extremely large amount of water into the upper atmosphere. Water vapor potentially saturated the atmosphere after impact, and might have destroyed O<sub>3</sub> via the HO<sub>x</sub> catalytic cycle (31), warmed the climate as a greenhouse forcing agent (32), and removed some of the other impact emission aerosols (21). Here we will emit  $7.5 \times 10^6$  Tg of water that includes contributions from vaporization, splashing, and subsequent forest fires (21, 38).
- **Halogens and NO<sub>x</sub>:** The impactor, seawater, and fires all likely contributed to a sharp increase in Cl, Br, I, and NO<sub>x</sub> shortly after impact, all of which can destroy O<sub>3</sub> (e.g., 31) and cause ocean acidification (e.g., 23). We will include all halogen and NO<sub>x</sub> emissions in our simulations, with  $1.1 \times 10^{14}$  Kg of Cl,  $4.8 \times 10^{11}$  Kg of Br,  $9.7 \times 10^9$  Kg of I, and  $3.1 \times 10^{13}$  Kg of N (38). In order to accurately simulate the system response to these emissions, we will add high NO<sub>x</sub> chemistry, aqueous reactions, and condensation of the halogens into WACCM4, which could prove useful for research beyond this proposal

- **CO<sub>2</sub>:** The amount of carbon released from the impact and its consequences remains poorly quantified. We will begin with a recent post-impact estimate based on leaf gas exchange principles, which suggests a CO<sub>2</sub> increased of 250 ppm (121). This increase generally agrees with a ~300 ppm CO<sub>2</sub> increase estimated from biomass burning (38), but is significantly higher than the ~50 ppm CO<sub>2</sub> increase estimated from the impact site (112). Our soot and temperature reconstructions, in combination with our ocean BEC modeling, will help constrain CO<sub>2</sub> emission across the boundary (see section 4.1.4 CO<sub>2</sub> Sensitivity Tests).
- **Sulfur:** The production of sulfates from the sulfur emission has the potential to block light from reaching the surface and produce acid rain (e.g., 14, 46; **Figure 7**). However, the magnitude of these effects depends on the interaction with other emissions. Here, our primary sulfur emission will be  $3.25 \times 10^5$  Tg from the impact site, based on the estimate of Artemieva et al. (112).
- **Thermal Pulse:** Theory suggests frictional heating by spherules from the Chicxulub impact caused a unique climate signature, with extreme heating in the upper atmosphere that calms towards the surface (e.g., 29, 89). Here, we propose heating the atmospheric column instantaneously at the time of impact using the energy emission estimates of Segura et al. (29). We will also include surface heating from widespread fires as in Bardeen et al. (21).

#### 4.1.3 Soot Sensitivity Tests

Our new soot measurements will provide valuable size and abundance information at several locations that we can use to directly inform our K-Pg simulations. We will compare our new soot data against a variety of emission scenarios to determine what amount, distribution, and duration of soot emission was most likely (**Figure 6**). Because most soot is removed from the atmosphere within the first two-years after emission (e.g., 21), we can get an accurate estimate of soot deposition with short duration simulations that are relatively inexpensive. We will begin by performing three simulations with July as the month of impact to determine the vertical distribution of coarse and fine soot in the atmosphere, with either 100% of coarse and fine near the surface, 50% of coarse and fine at the local tropopause, or 100% of coarse and fine at the local tropopause. Next, we will perform six simulations to look at the duration and timing of emission, including emission over the course of a day, week, and month occurring in either January or July. The soot emission scenario that best agrees with the soot measurements will serve as our preferred duration estimate. From there, we will explore the month of emission in greater detail with simulations during every month of the year. These experiments will shed new light on the controversial work attempting to determine the month of impact (160, 180). Overall, these experiments will determine the amount of biomass burned after impact. The soot emission scenario that best matches our and previous soot measurements will determine the emission configuration for subsequent simulations. In these soot sensitivity tests, other emissions will occur over the course of 1-day with amounts and locations coming from the estimates discussed above.

#### 4.1.4 CO<sub>2</sub> Sensitivity Tests

To better understand the full effects of CO<sub>2</sub> emitted after the K-Pg, we will perform four 1,000-year sensitivity tests. These CO<sub>2</sub> tests will include a no CO<sub>2</sub> emission scenario, an impact site only estimate (~50 ppm; 112), a leaf gas exchange estimate (~250 ppm; 121), and a biomass burning plus impact site estimate, which we will calculate from our new biomass burned analysis. These experiments will begin with a 50-year WACCM+CARMA simulation that represents our best estimate of all emissions from the Chicxulub impact event with the possible CO<sub>2</sub> estimates. Then, we will return to the low top model configuration (CAM4) to reduce computational costs and extend these simulations with interactive carbon cycling for an additional 1,000 years each. Here, we will manually adjust the terrestrial carbon to reflect biomass burning when appropriate, while the land model will handle the terrestrial carbon response to the impact winter (181). Likewise, the ocean BEC model will calculate the marine carbon flux post-impact. Online and offline calculations will be employed using data from the model experiments to estimate CO<sub>2</sub> drawdown after the impact. We will compare the resulting simulated temperatures with our new and previously published high resolution temperature reconstructions across the K-Pg. We will use the CO<sub>2</sub> emission scenario that best matches the proxy temperature reconstructions in our long duration simulation.

#### 4.1.5 Long Duration Simulations

Many records are unable to capture the geologically short-lived climate responses to the atmospheric forcings from the Chicxulub impact (e.g., 49, 65). Instead, long-term biological and chemical signals are

often used to infer the short-term forcings. Given the skew towards low temporal resolution in the geologic record, multi-millennial scale climate simulations are ideal. Therefore, we will run a low-resolution simulation for 50-kyr, using upscaled atmospheric forcings from the WACCM4+CARMA simulations.

We will begin with the 50-year WACCM4+CARMA simulation that represents our best estimate of all emissions from the Chicxulub impact event. Working from the sensitivity experiments described above, we will use the soot emission estimate that most favorably compares with the soot deposition records and the CO<sub>2</sub> emission estimate that best compares with our post-impact temperature reconstructions along with the sulfur, nano-particles, water, halogens, NO<sub>x</sub>, and atmospheric heating estimates discussed above. We will use the Chicxulub impact outputs from this simulation to provide 50-years of upscaled climate forcings for the low-resolution version of CESM with ocean BEC. We will then extend this low resolution simulation for 50-kyr without external forcings. We will prescribe CO<sub>2</sub> drawdown from silicate weathering based on an enhanced rate estimate from GEOCARB (182, 183). The carbon cycle code in CESM will allow for CO<sub>2</sub> fluctuations by the ocean in the long term simulation (154). We will hold the orbit fixed at preindustrial values, because orbital configuration is unknown beyond ~50 Ma (184) and the orbital variations will likely produce a signal secondary to the asteroid impact. The long duration simulation will allow for direct comparison with geologic records, helping us understand the mechanisms responsible for regional patterns of ocean biological response to the K-Pg extinction (36, 185) and the slow recovery of the δ<sup>13</sup>C vertical gradient (e.g., 14, 25, 186).

#### 4.2 Fish Debris and Organic Temperature Reconstructions

Two weeks of fieldwork in Denmark will occur in the first year of the grant. The goal will be to collect a stratigraphically complete sequence spanning 500 kyr before to 500 kyr after the boundary with cm scale or better resolution in the Fiskeler Member, as described above. In year two, we plan a trip to the Bremen Core Recovery to collect samples from the K-Pg boundary interval at ODP Site 1258, 1259, and 1260 from Demerara Rise (**Figure 3**) at cm-scale resolution spanning the same million-year interval straddling the boundary. Sample analyses will begin as soon as samples are returned to Columbia. For both outcrop and core samples, bulk material will be disaggregated, fine fractions will be collected and shared with PI Mitra for soot analyses. Microfossils will be picked from the coarse fraction, and their preservation will be documented with reflected light microscopy and SEM studies. Oxygen isotopic ratios of fish debris and foraminifera will be measured in PI MacLeod's lab at the University of Missouri following established methods (e.g., 33, 187). All new samples will be tested for the presence of GDGTs for the calculation of TEX86-derived temperatures.

#### 4.3 Soot Reconstructions

Using data collected from Stevens Klint, El Kef, Demerara Rise, and Caravaca, a few mg of bulk sediment will be subsampled for %OC and δ<sup>13</sup>C. Subsequent to that, the remainder of the sediment will be separated via heavy liquid flotation in sodium polytungstate at densities of 1.6, 2.0 and 2.5 g/cm<sup>3</sup>. After separating into size classes and washing, sediments will be sieved through 250-, 63-, and 38-μm stainless steel sieves. The dried residue will be subject to the CTO-375 soot isolation (127) in each size class. Finally, the soot isolate in each size class would be quantified for %soot C and δ<sup>13</sup>C<sub>soot</sub>.

#### 4.4 Biomarker Reconstructions

We anticipate analyzing samples from ~120 horizons only from freshly recovered samples and from sections that exhibit a low degree of thermal alteration and sufficient organic carbon content (i.e., Stevens Klint and El Kef coring Program; 122, 124). For samples where total lipid extracts are not yet available (i.e., Caravaca and part of El Kef) freeze-dried powdered samples will be extracted, cleaned, and separated into different lipid classes as described elsewhere (122). We will analyze aliphatic and aromatic hydrocarbons by gas chromatography-triple quadrupole-mass spectrometry (GC-QQQ-MS) using a Thermo Scientific Trace 1310 GC interphase to a Thermo Scientific TSQ 8000 EVO MS on both full scan and selective reaction monitoring (SRM) modes. We will analyze core GDGTs by high-performance liquid chromatography-high resolution mass spectrometry (HPLC-HRMS) using a Thermo Scientific Ultimate 3000 HPLC interfaced to a Q Exactive Focus Orbitrap-Quadrupole MS, following Hopmans et al. (188). Subsequently, ocean temperatures will be reconstructed using TEX<sub>86</sub> paleothermometry following Schouten et al. (123) and the transfer functions of Kim et al. (189) and Tierney & Tingley (190).

## 5 HYPOTHESIS TESTING

Here we summarize how our combination of model simulations and proxy reconstructions will address several often-debated hypotheses involving the end-Cretaceous mass extinction.

### H1: The Chicxulub impact caused widespread fires and soot emission, which was a primary contributor to the impact winter.

The magnitude of fires remains one of the most controversial aspects of the Chicxulub impact. There exist K-Pg records and model experiments to both support and refute the hypothesis that frictional heating from the deposition of recondensed ejecta caused an infrared radiation pulse capable of starting concurrent widespread fires, thus emitting large quantities of soot into the atmosphere (e.g., 27, 94, 98, 101, 103). Not only would the thermal pulse and resulting fires devastate life on land (30), but several recent modeling studies emphasize the potential importance of soot in causing impact winter (21, 22). Therefore, refined soot estimates are a critical first step for progressing our understanding of the end-Cretaceous climate and the associated extinction and recovery.

Our proposed data collection efforts will provide the first new measurements of soot deposition across the K-Pg boundary in over 17 years. From these measurements, we will refine the magnitude of soot emission, size spectrum of the soot particles, and the timing of the fires with respect to the boundary. New and continuing high resolution PAH and  $\delta^{13}\text{C}$  measurements from the same sites will further clarify the extent and timing of biomass burning. These data will become inputs for the Earth system model, which allows for the explicit evolution of soot particles of different sizes in the atmosphere, affecting global cooling (21). Sensitivity tests of injection height, timing, and duration of soot emission will provide prognostic simulation of soot deposition (**Figure 6**). Comparison of model simulated soot deposition with our new and previously published soot records will constrain the intensity of the thermal pulse, extent of fires, and characteristics of the impact winter. Our proposed long duration simulations well assess the significance of improved soot emission on the long-term recovery of ocean life.

### H2: CO<sub>2</sub> emission from the impact site and widespread fires resulted in several degrees of warming in the millennia after the Chicxulub impact.

The asteroid impact potentially led to an abrupt CO<sub>2</sub> increase (121), with emissions from vaporized carbonate rock (112) and biomass burning (38). Unfortunately, theoretical CO<sub>2</sub> emission estimates contain large uncertainties and proxy-based CO<sub>2</sub> reconstructions with the temporal resolution necessary to capture this abrupt signal are rare and debated (121, 191). Therefore, we propose to determine the post-impact CO<sub>2</sub> spike indirectly by producing a series of millennial scale or finer temperature reconstructions across the K-Pg. In combination with our new burning estimates, ocean biogeochemistry simulations, and previous high resolution temperature reconstructions (e.g., 33, 34, 49, 66), we will be able to provide an improved estimate of CO<sub>2</sub> emitted as a result of the Chicxulub impact, as well as the most likely source(s) of this CO<sub>2</sub>. Importantly, our model simulations will capture the spatial variability of the temperature response to abrupt CO<sub>2</sub> increase, which will be useful for understanding the variability found in current post-impact temperature reconstructions (15). Further, model simulated ocean biogeochemistry and vegetation regrowth will help determine the length of this CO<sub>2</sub> increase. A short atmospheric residence time could help explain the lack of warming found in some low resolution and deep-sea temperature reconstructions.

### H3: CO<sub>2</sub> and sulfur emission from the impact drove ocean acidification, which delayed the marine recovery and contributed to the loss of the $\delta^{13}\text{C}$ gradient.

Several studies suggest that ocean acidification played an important role in the marine extinction and recovery after the K-Pg (e.g., 14). However, many uncertainties remain about the driver(s) and magnitude of acidification, responses of the marine ecosystem, and impact on the isotopic signatures. As mentioned, our model-proxy comparison will determine an impact-generated CO<sub>2</sub> estimate. Additionally, the explicit aerosol resolving scheme within the atmosphere model (151) will determine the rate and concentrations of H<sub>2</sub>SO<sub>4</sub> and NO<sub>x</sub> deposition into the ocean using latest emission estimates from the K-Pg (38, 112). Our ocean biogeochemistry model (154) will calculate the marine pH and biotic responses to the influxes of CO<sub>2</sub>, H<sub>2</sub>SO<sub>4</sub>, and NO<sub>x</sub> (**Figure 7**). Further, inclusion of carbon isotope tracers in the ocean model (156) will allow us to determine the roles of impact-driven changes in ocean chemistry, production, and circulation on the long term reduction in the  $\delta^{13}\text{C}$  gradient (e.g., 192). Our new suite of high-resolution ecological biomarkers will also be directly comparable with our model outputs, providing additional constraints on the marine response in the millennia after impact. We anticipate that our results will continue to move the

community beyond the original “Strangelove ocean” hypothesis by highlighting the resilience of marine life.

#### **H4: Ozone destruction from Chicxulub impact emissions exacerbated the extinction and delayed the recovery by increasing surface UV exposure.**

A post-impact spike in UV associated with stratospheric O<sub>3</sub> destroying molecules, such halogens and NO<sub>x</sub>, is an underexplored K-Pg kill mechanism (31). Recent model developments allow for direct calculation of O<sub>3</sub> and surface UV response from the Chicxulub impact (21). Our preliminary results suggest that impact-driven emissions of halogens and NO<sub>x</sub> destroy a large percentage of stratospheric O<sub>3</sub> for decades, potentially exacerbating the extinction and prolonging the recovery. Part of this proposal will involve refining high NO<sub>x</sub> chemistry in the model to improve its atmospheric residence time. These efforts will compliment an ongoing project by Dr. Barry Lomax to determine post-impact changes in UV using sporomorph chemistry (193; see letter of collaboration). This collaboration will both clarify the complicated radiation responses found in his records and provide independent constraints on the duration of O<sub>3</sub> destruction associated with the impact. The findings will tie into our proposed model development on the marine plankton sensitivity to UV, which will quantify a previously unexplored, but likely significant, effect of the Chicxulub impact on the proxy record. Further, the ability to simulate ocean biogeochemistry / UV interactions has applications well beyond this study including the effects of UV increase from O<sub>3</sub> loss in the aftermath volcanic eruptions and nuclear conflict (194, 195).

## **6 BROADER IMPACTS**

### **6.1 Implications for Society**

The goal of understanding mass extinction and extreme climate perturbations is increasingly relevant as we head towards an uncertain climate future. Interpreting what led to the K-Pg extinction and how biota recovered can provide an analog for Earth’s current extinction trend. Simulation of the theorized abrupt increase in greenhouse gas concentrations across the K-Pg boundary, in particular, will help us quantify future climatic and biotic responses under similar forcings. Further, this work will provide valuable model development including high NO<sub>x</sub> chemistry in WACCM4 and marine plankton sensitivity to UV radiation, with applications beyond the K-Pg such as volcanic eruptions and geoengineering.

### **6.2 Human and Scientific Infrastructure Development**

If funded, this proposal will support three early career scientists (Clay Tabor, Cheryl Harrison, and Julio Sepúlveda), two postdoctoral researchers (one at UTRGV and one at CU Boulder), four PhD students (one at UConn, one at ECU, one at MU, and one at CU Boulder), one MSc student at UTRGV, and several undergraduate students. This proposal will not only advance their careers, but also promote continuing collaboration with the many universities involved in this project. Graduate student projects will involve proxy analyses, paleoclimate modeling, and ocean biogeochemistry and ecosystem model analysis, and model-proxy synthesis. All PIs will be encouraged to help mentor the graduate students; we will provide opportunities for laboratory exchanges so that students can learn from and interact with the PIs, as well as opportunities for students to be involved in education and outreach activities. Further, frequent in person and virtual team meetings will expose graduate students to a range of methods and techniques, as well as a number of role models, including two female scientists and one Latino scientist. The students will leave this project with a strong background in both geochemistry and Earth system modeling, which will position them well for future success. Undergraduate students will assist with model setup, analysis, and model-data comparison. We will sponsor undergraduate students for two years, starting in their junior year, with the goal that they present results at a high-profile conference during their senior year and contribute to and/or lead publications. We will seek out and encourage students from underrepresented groups to apply for these research opportunities, in particular through UTRGV, a Hispanic majority institution.

### **6.3 Integration of Education and Outreach**

This proposal will additionally support the participation of three underrepresented undergraduate summer interns via the Research Experiences in Solid Earth Science for Students (RESESS) program, housed at UNAVCO in Boulder, CO. RESESS is a paid research internship for undergraduate students with a mission of increasing diversity in the geoscience workforce. The overwhelming majority of RESESS alumni are members of underrepresented groups (93%), and over 80% of post-baccalaureate RESESS alumni are in geoscience graduate school or employed in the geoscience workforce. Students participating in the

RESESS program typically spend their first summer in Boulder, CO, working on an authentic geoscience research project and participating in multiple professional development programs. Interns returning in subsequent years typically work at the university of a community scientist, traveling to Boulder the first and last weeks of the program. All interns are supported to present their research results at a scientific conference within 12 months of the completion of the summer research experience. Our project team has committed to providing mentoring support and a research experience for three interns. It is expected that interns will spend their first year in Boulder, working under the supervision of PIs Lovenduski or Sepúlveda, with support from Harrison. If interns commit to repeated summers, they will have the opportunity to work under the supervision of the other project PIs at other institutions. PIs Lovenduski and Sepúlveda have successfully mentored RESESS interns in the past and have a good working relationship with the RESESS program. PI Harrison, who works at a majority (88%) Hispanic institution, will encourage the application of diverse students to the RESESS program. Furthermore, PI Sepúlveda plans to recruit 2-3 undergraduate students in financial need per year through CU's Work Study Program to work as laboratory assistants.

Mitra's ECU PhD student associated with this project will be recruited through ECU's Integrated Coastal Sciences (ICS) PhD program (formerly ECU's Coastal Resources Management PhD program), which has had a recruitment rate of 75% females and minorities over the past 5 years. The ICS program requires students to incorporate natural sciences with social sciences in their research. This doctoral student will incorporate either economics (costs of biological extinction) or human dimensions of impacts (avoidance risk behavior vs disaster intensity) into their dissertation research, in addition to the soot analyses from the proposed sites (geosciences). This portion of the project in particular will be key to rigorously investigating the societal implications of our findings.

Earth science education is becoming increasingly scarce at the K-12 level. Consequently, students often have little knowledge of potential career paths in Earth sciences before attending college. At MU, PI MacLeod proposes collaborating with Ms. Karen Hibdon and her AP Environmental Studies class at Hickman High School in a place-based (local students interfacing with work done at the University) and problem-based (a hands on, experimental experience with oxygen isotope paleothermometry) project aimed to give students a chance to better appreciate the observations and science that inform deep-time paleoclimate reconstructions. Students will determine the temperature dependence of  $\delta^{18}\text{O}$  values in inorganically precipitated calcite using a passive degassing approach, which will allow students to make solutions, monitor concentrations, manipulate pH, and change saturation state. Students will plot  $\delta^{18}\text{O}$  results versus temperature of the precipitation and calculate the temperature dependence of carbonate  $\delta^{18}\text{O}$  values from the resulting graph. Once they have developed their paleothermometer, the students will be given data generated in this study and asked to interpret the results relative to potential temperature change across the K-Pg boundary. This exercise will expose students to the actual techniques that scientists use, contextualizing their classwork within the drama of the K-Pg event, and encourage them to continue in STEM. Ms. Hibdon will also attend annual PI meeting in Boulder and work on developing lessons that provide context and background on the K-Pg boundary and deep time paleoclimate studies. These laboratory exercises and lessons will be disseminated and made available for other teachers to use on the Open Science Framework (OSF) site associated with the project.

In addition to the K-12 educational outreach above, we will partner with the Connecticut State Museum of Natural History (see letter of collaboration) to create an exhibit in the Geosciences building that highlights the findings of our research. The UConn Geosciences building is an excellent location to publicize the excitement, importance, and possible career opportunities within Earth sciences. The exhibit will be located in the building's main hall, which receives diverse foot-traffic (>1,000 students per semester) from largely early career college students. We will commission paleontology artist James Kuether to create a mural based on our simulations and proxy reconstructions that conveys the environmental catastrophe resulting from the Chicxulub impact. This image will be paired with information about the K-Pg mass extinction, how we are working to better understand its causes, and how it can help inform future environmental change.

Results will also be published through more traditional avenues. All significant research findings will be published in peer reviewed journals, with a preference towards open-access journals when possible. PIs and their students will also frequently attend professional meetings as a way to present their results and receive feedback from the community. Moreover, we will host select datasets on public archives for easy access by the community, and provide raw data upon request. Finally, PIs MacLeod, Tabor, Harrison, and Sepúlveda will incorporate the findings of the project into class lectures and discussions, including classes at UTRGV, a majority Hispanic institution.

## MANAGEMENT AND INTEGRATION PLAN

**1 Effort Coordination:** During the first summer of year 1, all PIs, postdocs, and graduate students will meet at CU-Boulder to discuss initial efforts. All PIs will briefly present their contributions to the project, including motivations, techniques, and outstanding issues. A group discussion on the top priorities for the coming years will follow. This meeting will conclude by creating a timeline for expected accomplishments, ranked by priority and significance to the overall project goal of understanding the K-Pg extinction. We will have additional meetings in Boulder, CO, in years 2 and 3 during which we will discuss progress, problems, and publications. During the 3<sup>rd</sup> meeting, we will discuss remaining tasks and potential areas for future research.

In addition to in-person meetings, we will promote video-chat discussions at least every three months to track progress and identify issues that might need attention before the next meeting. Further, we will encourage impromptu meetings to discuss interesting developments and major setbacks and meet at popular conferences such as AGU. Graduate and undergraduate students will be especially encouraged to participate and present research at these conferences, and travel has been budgeted to this end.

We plan to coordinate research efforts using several common organizational tools, including Google Calendar and Docs, Slack, Dropbox, and Open Science Framework (OSF). Moreover, we will store raw model data on a combination of the UConn and NCAR facilities. Frequently read model data will be housed on Network Attached Storage for easier access by the team. Smaller datasets will be housed in the team OSF site, which will eventually be used for data publication.

**2 Data Storage, Management, and Dissemination:** This project is a “big data” effort. We expect to generate over 75 TB of model data as well as a compilation of chemical, biological, and sedimentological data from decades of research on the K-Pg. Therefore, we will purchase a RAID configured Network Attached Storage to allow for consistent and rapid data access by all team members. For visualization and organization, we will use GIS to georeference the compiled data from our literature review, using locations consistent with the model paleogeography. We will utilize OSF to organize, and disseminate the K-Pg proxy record compilation, the new proxy data gathered, and selected model outputs. Select data of broad interest will also be submitted to scientific data archives such as WDS-Paleo.

**3 Research and Education Integration:** To involve secondary school students directly in the science, we will develop and implement a lab-based module at MU involving Hickman High School students in which they precipitate calcite at different temperatures to investigate whether there is a temperature signature in  $\delta^{18}\text{O}$  values. We will also develop an exhibit in UConn’s geosciences building in collaboration with the Connecticut State Museum of Natural History. Finally, at ECU, the graduate student will directly connect their K-Pg soot research with the economics or human dimensions of impacts and biological extinction through the Integrated Coastal Sciences PhD program in which each entering cohort is  $\sim>75\%$  female.

All PIs are strongly committed to moving diverse undergraduate STEM students forward into graduate programs by providing genuine research experience and mentorship. Thus, we budget for undergraduate assistance with an emphasis on recruiting typically women and minorities. Of particular note, this proposal will support the participation of three underrepresented undergraduate summer interns via the Research Experiences in Solid Earth Science for Students (RESESS) program hosted at CU Boulder. In addition, PI Harrison has budgeted for two undergraduate researchers during each year of the project, all who will come from the  $\sim 90\%$  Hispanic population of UTRGV. These students will have the opportunity to interact with all project PIs, use project results for graduate and undergraduate theses, and present findings at conferences. Furthermore, PI Sepúlveda plans to recruit 2-3 undergraduate students in financial need per year through CU’s Work Study Program to work as laboratory assistants.

## 4 Detailed Timeline

### 4.1 Year 1

**Modeling:** PIs Tabor, Lovenduski, and Harrison in collaboration with a postdoc at UTRGV will initialize the ocean BEC. This involves testing the ocean BEC and isotope models with Chicxulub forcings under present-day conditions. After testing and debugging, we will add BEC and isotope codes, along with any necessary modifications, to our previously equilibrated Maastrichtian boundary conditions and run these simulations for several thousand years to create equilibrium model configurations that are ready to use in our Chicxulub impact perturbation experiments. Simultaneously, PIs Bardeen and Tabor, in collaboration with a UConn graduate student, will perform several short Chicxulub impact forcing tests to implement high NO<sub>x</sub> chemistry and condensed phase halogens into WACCM4.

**Proxy:** PI MacLeod and a MU graduate student will travel to Denmark for two weeks of field work.

Deliverable products to the group are detailed characterization of organic components that we hope will include GDGTs in sufficient abundance for TEX<sub>86</sub> paleotemperature estimates and estimates of the average and variance among phosphate δ<sup>18</sup>O values during the late Maastrichtian and early Danian. PIs Mitra and Sepúlveda and their graduate students will analyze existing samples from Demerara Rise, Caravaca, and El Kef for ecological biomarkers, PAHs, and soot.

**Education and Outreach:** Protocols and lessons for the exploration of oxygen isotope paleothermometry at MU will begin in the first summer of funding. The collaborating teacher at the Hickman High School and PI MacLeod will experiment with approaches to setting up and running the precipitation experiments to learn timing and explore/experience potential pitfalls. During the first summer, PIs Lovenduski, Harrison, and Sepúlveda will work with RESESS student at CU-Boulder, while PI Sepúlveda will also recruit and train undergraduate students in financial need through CU's Work Study Program as laboratory assistants. PIs Tabor, MacLeod, Mitra, and Harrison, will collectively recruit several undergraduates to continue extractions of soot and biomarkers and work on model setup.

#### 4.2 Year 2

**Modeling:** The graduate student at UConn, with guidance from PIs Tabor and Bardeen, will run the proposed soot and CO<sub>2</sub> sensitivity tests using information from our new soot and temperature reconstructions. The postdoc and master's student at UTRGV will evaluate the ocean biogeochemical and ecosystem response to these forcings. PI Lovenduski will work with a postdoc at CU Boulder to implement marine plankton sensitivity to UV radiation in the CESM BEC codebase. Once implemented, idealized, short-duration sensitivity studies will be conducted with only the ocean component to evaluate the ecosystem response to code modifications. Once we are satisfied with the response function, we will couple the modified BEC code with the full earth system for the long term simulation. We will combine our model and proxy data within a standard database for visual and statistical comparisons by the group.

**Proxy:** PI MacLeod and a graduate student will travel to the Bremen Core Repository to collect new samples from K-Pg cores from ODP Sites 1258, 1259, and 1260 collected on Demerara Rise. Analyses of Danish samples will continue and processing and subsequent measurement of stable isotopic ratios of foraminifera from Demerara Rise will begin. PIs Mitra and Sepúlveda and their graduate students will analyze existing and new samples for soot and/or, ecological biomarkers (both ecology and PAHs). Year 2 will also be dedicated to the compilation of proxy data and to the completion of manuscripts.

**Education and Outreach:** At MU, work in the second summer will fix or refine previous lessons and experiments, add additional complexity, and consider generalizing the lessons to other topics important in paleoclimate studies. Also, using our new insights about the short-term environmental consequences of the Chicxulub impact, we will begin our collaboration with the Connecticut State Museum of Natural History to create an end-Cretaceous mass extinction exhibit in the geosciences building at UConn. CU-Boulder will again host a RESESS undergraduate student. If this is a returning intern, they will have the opportunity to work under the supervision of the other project PIs at their institutions. Furthermore, PI Sepúlveda will continue recruiting and training undergraduate students in financial need through CU's Work Study Program as lab assistants. The ECU student will formalize the social science portion of their dissertation research.

#### 4.3 Year 3

**Modeling:** Building upon our previous results, we will use our most likely impact forcings to perform a long-term (50 kyr) simulation of the Earth system responses to the K-Pg impact. Results from this long-term integration, in combination with our ecological biomarkers, SST reconstructions and other compiled data, will provide insight into biological recovery in the ocean after the K-Pg boundary. The results will provide many research avenues for the UConn and UTRGV graduate students and CU-Boulder postdoc.

**Proxy:** Efforts in year 3 will focus on maximizing data generation in intervals and/or locations where model results suggest empirical estimates might best distinguish among alternative model results. These efforts might include replication for anomalous samples, finer resolution studies at Stevns Klint or Demerara Rise, and/or generating low resolution results from new sites (hundreds of K-Pg sites have been studied and samples exist for many of them especially IODP samples) from different regions.

**Education and Outreach:** With most of our experiments completed, we will work to disseminate results through peer-reviewed publications, class and public lectures. Early in year 3, the research team will submit at least one proposal to chair a session on the K-Pg impact at a national meeting. The final summer of RESESS internship will take place at CU-Boulder. More so than in previous years, we expect to bring undergraduates to AGU.

## RESULTS OF PRIOR SUPPORT

**Lovenduski; OCE-1752724:** CAREER: A Change in the Forecast: Ocean Biogeochemistry Over the Next Decade, National Science Foundation, (PI Lovenduski), 6/18-5/23, \$799,914.

**Intellectual merit:** The project team is analyzing near-term (1-10 years) predictions of ocean biogeochemistry across the global ocean using output from the Community Earth System Model Decadal Prediction Large Ensemble.

**Broader impacts:** This project will provide underrepresented, undergraduate students with transformative research experiences in oceanography that pave the way to future graduate school admission.

**Publications to date:** Lovenduski et al. (2019), Gruber et al. (2019)

**Data Sharing:** This project makes use of output from the Community Earth System Model Decadal Prediction Large Ensemble, which is publicly available on the Earth System Grid (<https://www.earthsystemgrid.org/dataset/ucar.cgd.ccsm4.CESM1-CAM5-DP.html>).

**MacLeod;** EAR-1323444: Collaborative Research: Testing the Early Late Ordovician Cool Water Hypothesis, National Science Foundation, (PI MacLeod, University of Missouri; co-PI's: Leslie, James Madison University; Herrmann, Louisiana State University), 6/13–5/17

**Intellectual Merit:** This project examined geochemical, paleontological, and sedimentological changes across a proposed Late Ordovician cooling interval. In contrast to predictions of cooling models, we found no  $\delta^{18}\text{O}$  shift across the lithologic transition between “warm-water” and “cool-water” carbonate deposition, and we found evidence for slight warming across a positive  $\delta^{13}\text{C}$  excursion proposed to be the signature of organic carbon burial. Burial of organic carbon has been invoked as a mechanism to lower atmospheric  $\text{pCO}_2$  levels and force cooling. Over longer stratigraphic intervals, we found conodont  $\delta^{18}\text{O}$  trends indicate stable or slightly warming conditions in the 10 million years before the Late Ordovician glaciation and mass extinction. Neodymium isotopes, on the other hand, indicate water with the signature of rocks in Taconic orogen spread across the Mohawkian Sea associated with lithologic changes. Our findings explicitly contradict models invoking long term, gradual cooling during the Late Ordovician and implicitly suggest that the end Ordovician glaciation and extinction were geologically quite rapid and catastrophic events.

**Broader Impacts:** Several joint field excursions among the 3 participating Universities were supported. The grant supported 2 undergraduate theses and 4 undergraduate research projects at JMU, 3 undergraduates, 4 masters, and one PhD student at LSU, and MU PhD student (Page Quinton) who is now an Assistant Professor at SUNY Potsdam.

**Publications:** Refereed papers: Quinton and MacLeod (2014), Quinton et al. (2015a; 2015b; 2016a; 2016b; 2017), Hughes et al. (2015), MacLeod et al. (2017), Wright et al. (2017), and Quinton et al. (2018) [bibliographic information provided in the ‘References’ section]. Abstracts at national and international meetings: 14, including 2 undergraduate presenters and one keynote address.

**Mitra;** OCE 1902496: 2018 Hurricane Season: RAPID: Associated Priming of Carbon in the Albemarle-Pamlico Estuarine System (APES), the Mid-Atlantic Bight and Gulf Stream, (PI Mitra, Eastern Carolina University), 11/18-10/20, \$101,532.

**Intellectual Merit:** This study quantifies the biological and chemical impacts from the 2018 Hurricane Season to the North Atlantic Ocean. Because marine DOM is a highly complex and polydisperse mixture of different compounds, its priming and biodegradation resulting from the storms, even at rudimentary levels may potentially be a significant contributor to coastal DIC and  $\text{CO}_2$  fluxes. Results suggest high velocity associated 2018 rainfall deposition eroded and mobilized elevated amounts of terrigenous organic matter (particulate and dissolved), nutrients, and bacteria, into the Gulf Stream. Priming experiments are ongoing to determine how the storm season affected the carbon cycle in the Gulf Stream.

**Broader Impacts:** Carbon cycling and microbial community analysis in the APES and adjacent Gulf Stream ecosystem provides substantial evidence of ecosystem impacts from the 2018 storms. The project supports the 2 female undergraduates and one female M.S. Thesis. An outreach event on storms and their impacts on water quality was conducted at a local elementary school.

**Publications:** This work has produced 3 presentations at a regional meeting and 1 presentation at a national meeting. Data for this ongoing project are archived at ECU’s permanent institutional repository, DataVerse, at Joyner Library, and are available by contacting the PI. Upon project completion, all datasets from this project will be archived in the Biological & Chemical Oceanography Data Management Office (BCO-DMO) which can be accessed via the BCO-DMO website.

**Sepúlveda:** EAR-1338318: ELT Collaborative Research: Perturbation of the Marine Food Web and Extinction During the Oceanic Anoxic Event at the Cenomanian/Turonian Boundary. National Science Foundation (PI Sepúlveda, University of Colorado), 01/2015–08/2020, \$176,978.

**Intellectual Merit:** This project uses a multidisciplinary approach (paleontology, organic and isotope geochemistry, and biogeochemical modeling) to address marine ecosystem response to ocean acidification and widespread hypoxia across the Cenomanian/Turonian Boundary in the Western Interior Seaway at high temporal resolution. The insight gained from the CTB can be applied to other intervals of biotic upheaval in Earth's history and will help improve projections of the impacts of human activities on modern ecosystems.

**Broader Impacts:** At CU Boulder, where all the biomarker and compound-specific work is being carried out, this project has contributed to career development for one assistant professor (PI Sepúlveda) and trained one graduate student (Frank Boudinot), one minority undergraduate student through the UNAVCO RESESS summer program (Steven Moran, Wichita State University), one undergraduate honors thesis through NSF's Research Experiences for Undergraduates (REU) program (Jonn van Oosten, CU Boulder), and five undergraduate laboratory assistants through CU Boulder's Work Study Program.

**Publications:** This project has produced one published paper (Jones et al., 2019), and six published abstracts of oral and poster presentations by graduate student Boudinot, undergraduate student Moran, undergraduate student van Oosten, and PI Sepúlveda. Additionally, one manuscript is currently accepted for publication (Boudinot et al.), while two others are currently under preparation by graduate student Boudinot and the PI. Results from this grant were delayed by the set-up of the new lab of PI Sepúlveda at CU Boulder.

**Tabor;** AGS-1804747: Collaborative Research: P2C2-Multi-Time-Scale Climate Dynamics in California (CA): An Integrated Multi-Proxy Stalagmite, Monitoring, and Modeling Approach, National Science Foundation, (PI Montanez, University of California at Davis, co-PI Tabor), 9/18-8/21, \$133,319.

**Intellectual merit:** This project looks to better understand hydroclimate variability of Southwest North America by generating a set of multiproxy calcite and fluid inclusion records, resolved at the sub-decadal to centennial-scale, for stalagmites from Sierra Nevada, CA since the last deglaciation. The speleothem records will be interpreted within the context of many other paleoclimate reconstructions in the region and through comparison with a series of model simulations that track water isotopic change during key intervals of the past 21 kyr. The modeling component, led by Tabor, has already contributed to multiple presentations by the graduate students involved in the project.

**Broader impacts:** The project will help integrate under-represented high school and undergraduate students into geosciences research by 1) bringing students into the Vertically Integrated Project at UC Davis, which includes seminars, peer-mentoring, and team-based research in cave-monitoring, 2) developing a climate science-based curriculum for Vacaville (CA) High School, a Hispanic serving institution, and 3) creating an interactive cave exhibit involving a virtual reality research tour and 3-D stalagmite reconstructions. In addition, this project provides support for a graduate student.

**Publications:** So far, no peer reviewed publications have been completed under this project, but several publications are in preparation. Also, this work has produced nine published abstracts of oral and poster presentations at national and international conferences.

**Bardeen** – no prior NSF results  
**Harrison** – no prior NSF results