# Seed Funding: Building a Community for Reactive Flow Software Infrastructure

## 1 Overview

Stars have complex lives. They generate energy by fusing light elements into heavier ones and are responsible for producing every element heavier than helium in the Universe. Eventually, they run out of fuel and can undergo spectacular explosions or complex interactions with companion stars. We model the state of a star using the equations of hydrodynamics. Understanding the lives of stars requires building sophisticated simulation codes that solve the equations of hydrodynamics along with a variety of other important physics that all work in unison to produce a virtual model of a star.

Our research group has been developing software and algorithms for efficiently modeling stellar explosions on leadership-class supercomputers for almost two decades. During an explosion, reactions will alter the flow in the star (e.g., heat release will cause expansion, driving the temperature down) and the reactions will respond to the changing thermodynamic conditions. It is essential that the algorithm strongly couple the reactions to what the hydrodynamics is doing, in order to get an accurate model of reactions in a star. Most of the simulation codes in the community update hydrodynamics and reactions independent of one another (a technique called operator splitting). A key innovation in our codes is how we deal with reactions—we've spent the past five years developing methods that strongly couple hydrodynamics and reactions, such that the reactions respond instantly to the changes in the hydrodynamic flow. We've had great success using our tools to model stellar explosions, and have shown our methods are much more accurate than the operator splitting techniques in the community. Our research on these algorithms has been supported by the Department of Energy since 2006. Notably, all of our simulation codes are freely available online for anyone to see. This is important both for reproducibility and also to support the community and foster new collaborations.

Of interest to this seed funding proposal, we develop two libraries that make it easy to design a reaction network suited to a particular astrophysical problem (pynucastro) and to couple that network to a multiphysics simulation code (Microphysics). Other research groups, both within and outside of astrophysics have started to express interest in using these libraries. While we have already been able to help some groups make use of them, there is more to be done. We want to expand the reach of our libraries by generalizing their assumptions to work across a wider range of codes, both within and outside of astrophysics (e.g. terrestrial chemical reactions).

This seed funding is key to bootstrapping this project. Through the seed funding period, we will reach out to the groups we've been in contact with and work on modifying the library and do the "proof-of-concept" demonstrations that our libraries can work in other codes. We will also finish the key publication describing the Microphysics library, which will detail the methods we use. Together, this will allow us target a funding proposal through the NSF Cyberinfrastructure for Sustained Scientific Innovation (CSSI) program that will enable us to support the community using our libraries. We expect that the collaborations enabled here will also allow us to attract larger collaborative grants in the future as well.