

July 11, 2019

XSEDE

Extreme Science and Engineering
Discovery Environment

ECSS NIP Can Assist Xperts

Sergiu Sanielevici, NIP Manager, Deputy
Director ECSS

sergiu@psc.edu

NIP Mission

Novel and Innovative Projects (NIP) accelerates research, scholarship, and education by new communities that can strongly benefit from the use of **XSEDE's** ecosystem of advanced digital services. The NIP team helps to identify scientists, scholars and educators **from disciplines** that have not yet made significant use of advanced **computing** infrastructure, who are committed to projects that require **XSEDE** services and are in a good position to use them efficiently. NIP staff provides mentoring to these projects, helping them to **obtain XSEDE allocations** and to use them successfully.

Expanded Scope

- XSEDE ecosystem of advanced digital services: ***can include all providers.***
- NIP can help to advise and assist scientists, scholars and educators from ***any discipline whose projects include non-traditional workloads, specifically large, complex data analysis. Non-exclusive, editable list of Keywords to trigger NIP referrals:***
<https://docs.google.com/document/d/1cOe9wHjCJ3W6nComiUjFMcA-slhhNyRbkaQ9uFhgyVA/edit>
- NIP assistance is ***not limited to*** obtaining and successfully using XSEDE allocations.

NIP Activities

- ***Outreach and generating new projects:*** send speakers to events on campuses (in-person or remote), to conferences etc. In cooperation with the ECSS Training, Education and Outreach and the XSEDE Broadening Participation teams.
- ***Lightweight consulting:*** advise potential or new users on suitable resources, how to get access, how to write proposals etc.
- ***Mentoring:*** help to address problems that come up during project execution, including obtaining ECSS for XSEDE allocations.

NIP Team and Friends

- Currently 12 XSEDE funded staff (~5 FTEs) from PSC, SDSC, TACC, IU, NCAR and www.shodor.org
- Expertise in HPC, data analysis, ML/AI, visualization, containers, gateways, bioinformatics, digital humanities & social sciences, software engineering etc.;
- Members also work in other ECSS and XSEDE areas and at their SPs, so they can mobilize additional expertise and help as needed;
- NIP works with Domain Champions (influential practitioners) in genomics, economics, GIS, humanities, biomedical imaging.

“If we don’t know the answer we know whom to ask – and they will get back to us!”

Challenges of non-traditional projects

- Clarity of mapping between research goals and computational means
- Data
 - What data?
 - Digitization
 - Copyright, etc.
- Code
- Technical skills

How do NIP Experts help?

- Start by refining a project idea with the researchers/scholars, aiming to overcome the above challenges.
- Result: extract and document clear computational objectives and requirements.
- Bring in appropriate Xperts: specialists in the software, tools, and resources most likely to meet the project's needs.
- Catalyze a feasible project plan: What pays off for everyone? What does everyone bring to the table?
- Can stay involved throughout project execution.

Example: Paleoanthropology

- Curtis Marean, Principal Investigator
 - Foundation Professor and associate director, Institute of Human Origins, School of Human Evolution and Social Change, Arizona State University, Tempe AZ
 - Honorary Professor, Centre for Coastal Palaeoscience, Nelson Mandela Metropolitan University, Port Elizabeth, South Africa
- Eric Shook, co-PI and XSEDE Domain Champion (GIS)
 - Assistant Professor, Department of Geography, Environment and Society, University of Minnesota, Minneapolis MN
- David O’Neal, XSEDE ECSS Consultant
 - Senior Scientific Specialist, Pittsburgh Supercomputing Center, Carnegie Mellon University, Pittsburgh PA

Formal Paleoscape Model

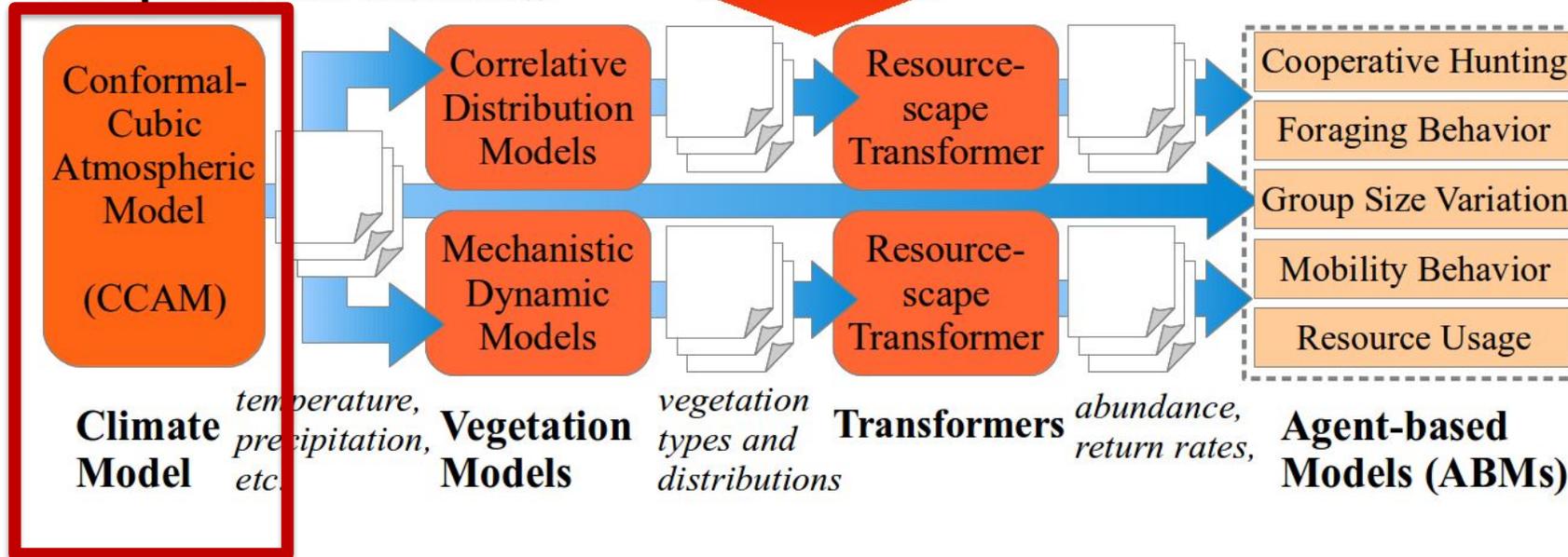
- A temporally dynamic model that projects resources meaningful to a hunter-gatherer
 - Structural Component
 - precise estimates of coastline distance
 - Food Availability Component
 - Where are the shellfish, bulbs, the seeds, and *what are their return rates?*
 - Techno-Resource Component
 - Where are the raw materials for flaked stone, ochre, etc.?
- Use it to create quantifiable hypotheses of human behavior through agent based modeling guided by the principles of behavioral ecology

Paleoscape Model Workflow

Climate States

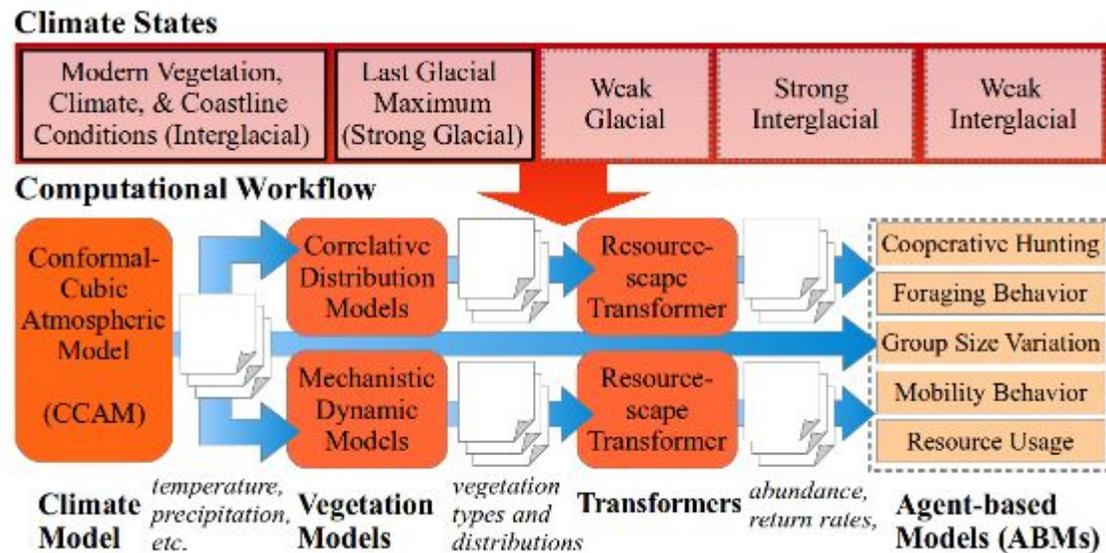


Computational Workflow



Workflow / Coupling Models

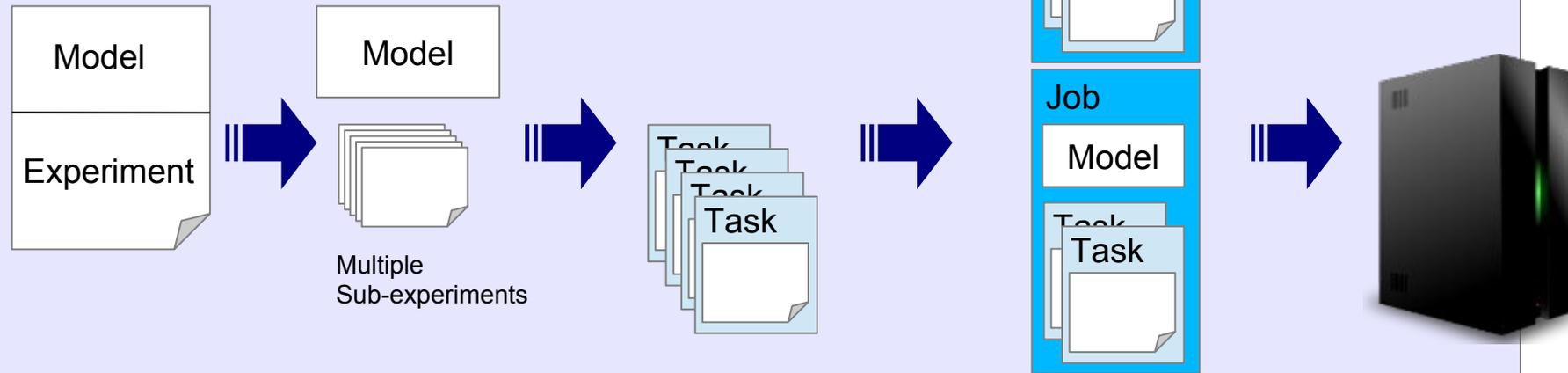
- Eric is developing a new domain-specific language for spatial-temporal data processing that will help couple the models
- It will transform the output from CCAM to be at the appropriate spatial and temporal scale and file format for the vegetative models.
- It will also be used for the Resource-scape Transformers



NetLogo ABM Workflow System (NAWS)

A NetLogo model file defines (1) an agent-based model and (2) (optionally) an experiment consisting of parameters for thousands of simulations

Open-sourced code available at :
<https://github.com/HPCGISLab/NAWS>



`parse-experiments.py`

Decompose an experiment into multiple sub-experiments

`generate-tasks.py`

Generate a task for each sub-experiment

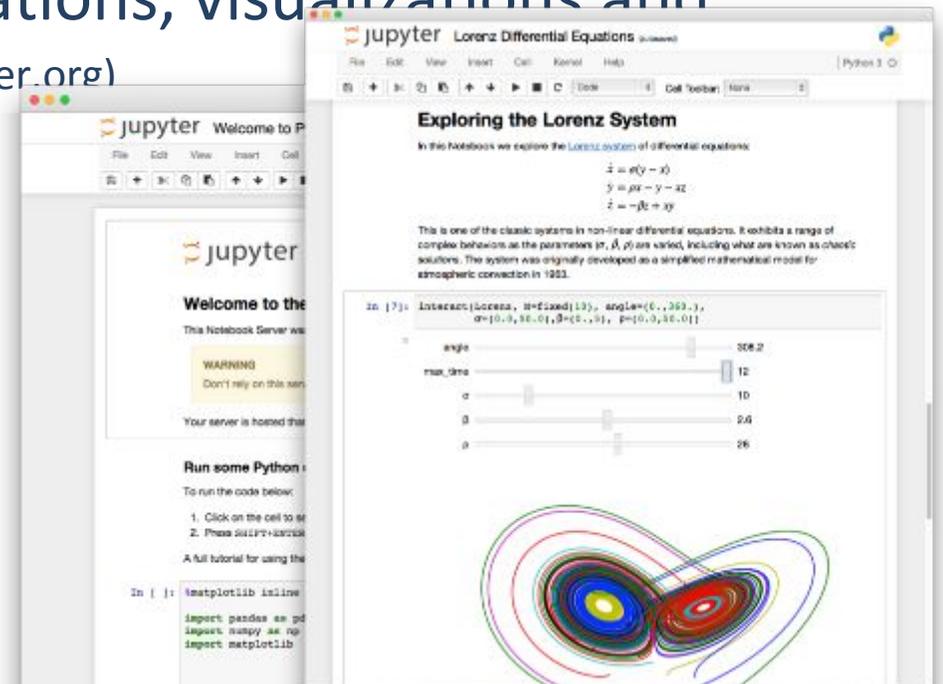
`submit-tasks.py`

Group one or more (multi-threaded) tasks into a job and submit to queue

Pilot Testing Jupyter Notebooks on Jetstream

- **Jupyter Notebooks** “open-source web application that allows you to create and share documents that contain live code, equations, visualizations and explanatory text.” (Jupyter.org)
- Exploring Notebooks as the UI for Paleoscape
- Davide Del Vento from NCAR Computational & Information Services Laboratory is leading the deployment of Jupyter on Jetstream

Image source: Jupyter.org



Example: Electronic Music

- **DISSCO** Digital Instrument for Sound Synthesis and Composition: PI Sever Tipei, University of Illinois; ECSS experts Paul Rodriguez, SDSC and Alan Craig, Shodor.
- Started by NIP, currently an ESRT project on SDSC *Comet*.
- For a composition that uses microsecond sampling and ~335K sounds generated for an 8 minute piece, end-to-end processing time was reduced from over 10 hours on the PI's workstation to about 3 hours on 16 nodes of *Comet*.
- This pioneering application of advanced computing to electronic music composition should inspire other creators in this and related communities (sonification, signal processing, etc.) to become adopters.

Example: Urban Traffic Analysis

- Urban Traffic Analysis : PI Jose Moura, CMU; NIP expert Paola Buitrago, PSC.
- Estimating vehicle count at intersections in a city is severely challenged by vehicle scale variations. Camera perspective variations make the generalization from labeled cameras (source) to unlabeled ones (target) highly non-trivial.
- With NIP expert help, on *Bridges GPU* and *GPU-AI*, the team has implemented a deep neural network to automatically learn camera perspective and adapt the counting model to unlabeled target cameras with perspective alignment. Extensive experiments on both vehicle and highly occluded crowd datasets verify the efficacy of the proposed methods and show significant improvement compared to the state of the art methods.
- Deep neural network research, both at the fundamental level and applied to a broad and rapidly expanding range of research problems in all fields of science, engineering, healthcare, scholarship and education, is a primary driver of the advanced computing and data intensive ecosystem. NIP and ECSS prioritize support of this aspect of the NSF's "Harnessing the Data Revolution" Big Idea.

We want to help you to help your users!

- **Check out our list of Keywords to trigger NIP referrals:**
<https://docs.google.com/document/d/1cOe9wHjCJ3W6nComiUjFMcA-slhhNyRbkaQ9uFhgyVA/edit>
- When your team comes across a user or project that fits this bill, and you feel they may need additional help, just send me email: sergiu@psc.edu
- I'll promptly get back to you and/or the researcher to organize an appropriate NIP activity.
- **Questions please!**