Nonlinear paths: career perspectives with a PhD in Math

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DMS, NJIT

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Outline

Intro: What I do now

CliMA Earth System Model Several challenges My main contributions Flux limiters for transport problems



2 How did I get here?

My background PhD project Internship project Postdoc project



Resources

Conferences and Association Resources **US-RSE** Tips Conclusions



Context / Motivation

The Climate Modeling Alliance (CliMA) is a coalition of scientists, engineers, and applied mathematicians from **Caltech**, **MIT**, and the **NASA Jet Propulsion Laboratory**. We are building the first Earth System Model (ESM) that automatically learns from diverse data sources to produce more accurate climate predictions with quantified uncertainties.



Context / Motivation

Temperatures have risen over the past 150 years



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Harnessing big data



Source: NASA - The Afternoon Constellation



Earth System Model



Targeted High-Resolution Simulations

Source: courtesy of Tapio Schneider

An Earth System Model (ESM) couples several separate components (Atmosphere, Ocean, Land. etc). In addition to this, we use Data Assimilation and Machine Learning to inform these models with more accurate parametrizations for subgrid scale phenomena.



Different Scales

For instance, a limited-area simulation can be nested in a global model and can, in turn, inform the global model.



Source: Physics Today - June 2021, pg. 44-51

Thousands of high-resolution large-eddy simulations (LES) can be embedded in a global circulation model (GCM) in a massively parallel computing environment (HPC clusters or cloud services), and the global model can learn from them.

Subgrid Scales

We can simulate some processes (e.g., clouds) faithfully, albeit only in limited areas.



Large-eddy simulation of tropical cumulus.

Source: Simulation with PyCLES (Pressel et al. 2015)

Open-source community project



Operators

Operators

Operators can compute spatial derivative operations.

· for performance reasons, we need to be able to "fuse" multiple operators and

function applications

I have worked in adding support for

- different "cubed-sphere" meshes:
 - Equiangular
 - Equidistant
 - Conformal
- high-order differential operators and flux limiters



- unit tests, integration tests and examples
- docs

🖓 Edit on GitHub 🛛 🕸

Shallow-water equations

The shallow water equations (in *vector invariant form*):

$$\frac{\partial h}{\partial t} + \nabla \cdot (h\boldsymbol{u}) = 0 \tag{1a}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + \nabla (\boldsymbol{\Phi} + \frac{1}{2} \|\boldsymbol{u}\|^2) = (\boldsymbol{u} \times (\boldsymbol{f} + \nabla \times \boldsymbol{u}))$$
(1b)

where f is the Coriolis term and $\Phi = g(h + h_s)$.

Written in terms of a curvilinear, non-orthogonal basis:

$$\frac{\partial h}{\partial t} + \frac{1}{J} \frac{\partial}{\partial \xi^{j}} \left(h J u^{j} \right) = 0$$
(2a)

$$\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial \xi^i} (\Phi + \frac{1}{2} \|\boldsymbol{u}\|^2) = E_{ijk} u^j (f^k + \omega^k)$$
(2b)

@. begin

end

Shallow-water equation Test Cases

ClimaCore.jl/examples/sphere/shallow_water.jl





Shallow-water equations suite, Test Case 5 [Williamson et al 1992]. Zonal flow over an isolated mountain. Shallow-water equations suite, barotropic instability test case [Galewsky et al 2004]. Zonal jet with compact support at mid-latitude. A small height disturbance is then added, which causes the jet to become unstable and collapse into a highly vortical structure.

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Examples: Flux limiters for advection (transport) problems

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \rho \boldsymbol{u},\tag{3a}$$

$$\frac{\partial Q}{\partial t} = -\nabla \cdot Q \boldsymbol{u},\tag{3b}$$

Transport of a passive tracer, with $Q = \rho q$, where q denotes tracer concentration (i.e., mixing ratio or mass of tracer per mass of dry air, in dry problems, or tracer mass per mass of moist air, in moist problems) per unit mass, and ρ fluid density.

@.	ystar.ρ = -wdiv(y.ρ * u)	#	contintuity	equatior	n
@.	ystar.pq += -wdiv(y.pq * u)	#	adevtion of	tracers	equation

Traditional SEM results are quite oscillatory for advection-dominated problems. Hence, we want to apply a local element reconstruction for the mimetic SEM formulation which yields an efficient quasimonotone (i.e., monotone w.r.t. the spectral element nodal values) limiter on *q*. This involves solving a constrained optimization problem (a weighted least square problem) that is local to each element [**Guba et al 2014**].

Flux limiter Test Cases: 2D sphere

 $ClimaCore.jl/examples/sphere/limiters_advection.jl$

p = 6, $ne = 20 \times 20 \times 6$ (effective resolution 0.75° at equator.)







With limiter.

Flux limiter Test Cases: 3D sphere

ClimaCore.jl/examples/hybrid/sphere/limiters_deformation_flow.jl

p = 4, horiz_ne= 4 × 4 × 6, vert_ne= 36







With limiter.

Some of my background: My Master thesis

Catmull-Clark subdivision of a closed surface.

Catmull-Clark subdivision of an open surface.

PhD project

Some of my background: My PhD thesis



Dewetting viscoelastic thin films.

Spreading viscoelastic drops.

Some of my background: Internship at Pixar



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Postdoc project

[SIAM-CSE] Postdoc Position at CU Boulder: High order discretization, multilevel methods, performance portability 🔅 🖶 🗵

Esterni > Posta in arrivo ×



Jed Brown jed@jedbrown.org tramite siam.org a slam-cse, slam-sc *

CU Bodet Computer Science has an immediate opening for a postdoctoral researcher in the development of robust and efficient methods for high order/compatible PDE discretization and multilevel solvers, including deployment in open source literaties. The project is especially interested in strategies to provide performance potability on emerging interested in strategies to provide performance potability on emerging solution in the strategies and provide performance potability on a merging solution in the strategies and potability of the solution in the strategies and variety of applications areas including sustainable energy and geophysics.

Successful applicants will have experience with PDE discretization, scalable algebraic solvers, and high-performance computing, with an interest in developing high-quality community software. Effective written and verbal communication skills will be needed to collaborate effectively with a distributed inter-disciplinary team and to disseminate results via publications and presentations.

Applications received by April 10 will receive full consideration and the position will remain open until filled. Apply here:

https://cu.taleo.net/careersection/2/jobdetail.ftl?job=13007

SIAM-CSE mailing list To post messages to the list please send them to: <u>SIAM-CSE@siam.org</u> http://lists.siam.org/mailman/listinfo/siam-cse lun 26 mar 2018, 13:10 🦙 🕤 🚦

Postdoc project (cont'ed)

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Website

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Office Hours

Varies by semester

Let was raised by wolves in a remote part of interior Alaska. Not surprisingly, his high-school mascot was a Wolfpack, but he deficient on longe and semed All American honors in cross-country sking while racing for the Nanols (hints of polaber) at the University of Alaska Fairbanks. Always fond of cold places, he wrote the Parallel (ce Sheet Model (PISM) while at UAE, and later eamed a Dr.S.: at ETI 42 zinch investigating computational methods for ice aheat and qlacier dynamics. Cardually warming our to temperate climates, he won the 200P Polet d'Or climating award for the first ascent of

Xuelian West in China's Tien Shan and has subsequently solved high-temperature problems while at Argonne National Lab. He has been a developer of the Portable Extensible Toolkit for Scientific computing (PETSG) since 2008. He was Asst. Computational Mathematician at Argonne prior to joining the faculty at the University of Colorado Boulder in 2015. His work has been recognized by the 2014 SIAG/SC Union's Scientist Price and 2014 IEEE TCS Vong Achiever Award, and as correspinent of the 2015 SIAM/ACM Prize in Computational Science and Engineering.



Postdoc project (cont'ed)





















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Conferences and Early-Career Programs

SuperComputing Early Career Program (ECP)

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US-RSE

US-Research Software Engineer Association: Website



RSE, and those who may not be RSEs but consider themselves RSE "allies" or manage individuals in RSE roles

Read More

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US-RSE (cont'ed)

US-Research Software Engineer Association: Slack



But what is a Research Software Engineer?

nature

Explore content v About the journal v Publish with us v Subscribe

nature > career q&a > article

CAREER Q&A 31 May 2022

Why science needs more research software engineers

Ten years after their profession got its name, research software engineers seek to swell their ranks.

Chris Woolston



A delicate balance

How much Research Vs Software Engineering you get to do depends on a multitude of factors





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Software Engineering Tips

- Try to do internships (either in national labs or industry)
- Try to contribute to open-source community software projects

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Summary and Purpose	_
IbCEED provides fast algebra for element-based discretizations, designed for performa-	100

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Tips

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Computational Science Tips

What skills do I need?

- Adopt best practices in your day-to-day work:
 - Version control: Use it to keep track of changes in your code and go back when you mess-up
 - Documentation: at the very least comment your code extensively
 - Organization: Good book-keeping of your numerical experiments (simulations, post-processing plots, etc)
 - Reproducibility: how do you respond to Reviewer 2 months later or to a random email writer years later?
- Try to adopt some software design patterns and engineering principles (e.g., test-driven design, unit testing, continuous integration)

General Tips

- Go to conferences, workshops, summer schools
- Talk to people
- Have a well-maintained online presence
- Apply early if you can
- Subscribe to associations' memberships and newsletters (SIAM is free for students!)
- Seek help, find mentors (not necessarily your thesis advisor)
- Some associations dedicated to minorities and their allies (e.g., AWM, WHPC)
- Use services available to you to overcome additional challenges such as impostor syndrome

Conclusions



It's ok to have nonlinear, zig-zagging paths.

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Conclusions



It's ok to have nonlinear, zig-zagging paths.



Just don't let it be this.



Questions?

Questions?

Thank you!



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NJIT Alumna Talk 2022

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