

My computational astrophysics journey

(before/during/after UBC)

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PhD with Douglas in 1995-1999



- Thesis: “Calculating the inhomogeneous reionization of the Universe”
- My journey started a little before that
- Computational astrophysics: running **first-principles** numerical simulations to model astrophysical systems, i.e. solving the underlying equations of (magneto) hydrodynamics, gravity, radiative transfer, ...
 - not semi-analytical models
 - not using ML to make up data

Start of the journey

- Always enjoyed calculating things + interest in stars
- First application: spherical astronomy

$$\begin{aligned}\sin h &= \sin \delta \sin \phi + \cos \delta \cos \phi \cos(LST - RA) \\ \sin A \cos h &= -\cos \delta \sin(LST - RA)\end{aligned}$$

- coolest thing: combined logarithmic trigonometric tables at 1' resolution, published around the turn of the 20th century \Rightarrow no need for a calculator

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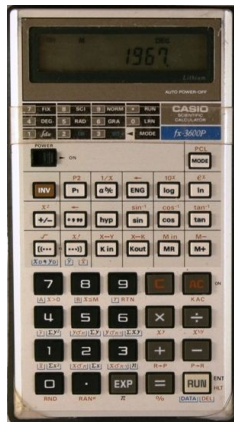
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- Went through the observational stage: built 1.5 telescopes, but did not really use them, especially with light pollution in the big city
- Computational: can build ever more sophisticated digital models of existing objects \Rightarrow infinite possibilities

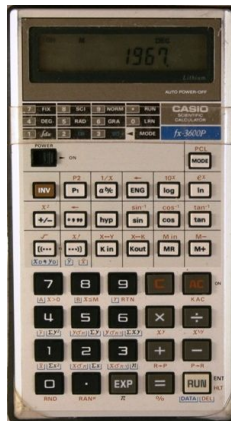
First missing element: hardware

- CASIO FX-3600P programmable calculator: my first serious tool
 - 38 steps of programmable memory
 - a digit key press counts as one step
 - Douglas only other person with the same model



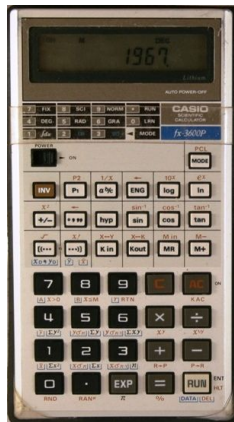
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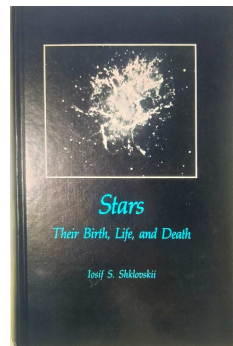
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- Fall 1986: managed to secure 1 hour / week with on a Yamaha PC clone with BASIC



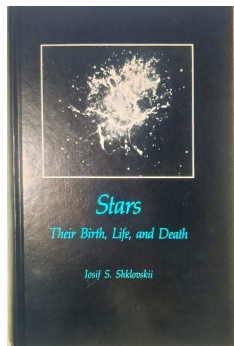
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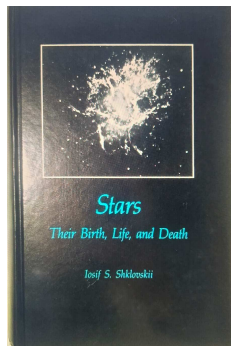
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- Just consider the forces acting on a body \Rightarrow update acceleration and velocity \Rightarrow trajectory over time
 - couple of examples
 - can apply the same to continuous fluids (equations of conservation)



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- Just consider the forces acting on a body \Rightarrow update acceleration and velocity \Rightarrow trajectory over time
 - couple of examples
 - can apply the same to continuous fluids (equations of conservation)
- Fall of 1986: started building a star formation model
 - spherical symmetry, break cloud into shells, compute forces on each, compute accelerations and velocities
 - another inspiration: Moscow planetarium children's courses taught by university graduate students (Jeans length in grade 7)
 - no clue about the Courant condition \Rightarrow quickly ran into numerical problems (no free lunch)
 - remained puzzled about the radiative losses
- In April 1987 submitted "Numerical modelling of molecular cloud fragmentation and collapse" technical paper



Moscow University: 1988-1994

- Choice between Faculty of physics (astronomy) and Faculty of Computational Mathematics and Cybernetics
 - awesome experience, rigorous math/physics/astronomy training, including PDE theory
 - however, no exposure to formal numerical techniques
 - arrested for walking on the observatory grounds at night \Rightarrow confirmed the suspicions about my observational career prospects + overexposed a set of photographic plates

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- 4th-year thesis: extracting energy from a rotating black hole
 - computing photons paths (null geodesics) in the Kerr metric
 - inject a photon into the ergosphere, let it split in two, one of them falls into the BH, the other can be captured at ∞
 - had trouble with accurate integration, in the end switched to processing some observational data

- 6th-year thesis: simulating accretion disks around compact objects
 - wrote my first proper hydro code: approximate Roe solver on a 2D grid
 - in the process learned Lagrangian and Eulerian methods, grid- and particle-based techniques, conservation schemes and Godunov's methods, Riemann solvers, compressible supersonic CFD
 - blew the power supply in my advisor's PC when I plugged it into a 220V outlet
 - spent few nights building an electric transformer from scrap wire
 - still was officially labelled fire hazard \Rightarrow the rest of my thesis computing was done in an unheated roof shack on top of the astronomy institute in December 1993 - January 1994

UBC: early years (1994-1996)

- Did not care about the topic, but wanted to compute
- Started looking into illumination in LMXBs with Jason Auman problem
 - ☞ connected to the previous problem
 - a “perturbed” stellar structure code?
 - a large range of scales: thermal time, rotation time, convection time (hours to months)
 - played with SPH, but ultimately decided to write an implicit hydrodynamics code, hoping to get away with larger timesteps
- My first introduction to large-scale numerical linear algebra
- The need to compute illumination from the compact object brought me to numerical radiative transfer

Computational astrophysics branches

1. Trivial: N-body (simplest possible computational problem)
2. One step up in difficulty: compressible fluid dynamics (well-established field, still many opportunities)
3. Another step: MHD
4. More difficult: radiative transfer and RHD
5. Standalone: numerical relativity, broad range from working in a given metric (dipped my toes in this twice) to solving the Einstein's field equations (0 experience)

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~1996: started thinking how to implement numerical RT in a hydro code

May-June 1996: one month at CITA

~1997: conversations with Douglas \Rightarrow things fall into place for doing a thesis on reionization

Numerical radiative transfer – why is it so hard?

1. 6D + time
2. Light travels at the speed of light
3. At large τ tight coupling with matter
 - static: incorrect computation of sources and sinks \Rightarrow wrong speed of fronts, e.g. I-fronts
 - scattering (static or moving) \Rightarrow slow convergence
 - moving: aberration, advection, Doppler shift, etc.
4. Problems with parallel decomposition (more on this later)

Solutions circa 1999

- Symmetries to reduce dimensionality
- Invest into better spatial/angular discretization
 - long vs. short characteristics
 - moment methods, Eddington factors with some closure scheme
 - Monte Carlo? (but only if you are lazy)
 - 5D/6D grid-based Boltzmann solvers
 - coupled RHD Riemann solvers for simple standard problems, e.g. spherical radiation-driven explosion, and stitch your solution out of these
- Post-process without hydro
- Best in coupled RHD: write all terms as expansions in $O(v/c)$ and throw away smaller terms
 - pioneered for stellar atmospheres and winds by D. Mihalas in (1+1+1)D
 - repeated for some simpler geometries by other authors
 - ideally need to do the same in (3+2+1)D

⇒ “Calculating the inhomogeneous reionization of the Universe”

static RT solver on a 128^3 Cartesian grid, 3 frequency bands, coupled with a custom time-dependent chemistry solver

1st postdoc: continue to work on RT in galaxy formation context

1999-2003 with Michael Norman at UIUC and UCSD

- (1) working to improve my RT solver
 - (2) putting it into Enzo (block-structured AMR galaxy formation code) ✗ not proper RHD
- Started to work with MPI-parallel codes
 - Quickly discovered that parallelization/decomposition is different for local (hydro) vs. long-range (RT) physics
 - RT speed was a big issue holding the entire code back (more on this later)



2nd postdoc: neutrino transport in core-collapse supernovae

2003-2006 postdoc with Anthony Mezzacappa (and the Terrascale Supernova Initiative) at ORNL

- Neutrino transport ($\rho \gtrsim 10^{14} \text{ g/cm}^3$) in GenASiS (General Astrophysical Simulation System)
 - cell-based AMR, F90/95, 6D coupled special relativistic MRHD with self-gravity and full Boltzmann transport
 - distributed MPI code with some PGAS features for storing neutrino-matter interaction coefficients
 - PETSc for linear solvers
- Responsible for:
 - neutrino emission and absorption
 - neutrino-matter scattering
 - neutrino-neutrino pair interaction (and neutrino flavour oscillations)
 - multi-dimensional neutrino tables implemented with Global Arrays
 - Riemann hydro solver for the nuclear equation of state
- Wonderful team of 5-6 people, but this was really a monumental project requiring hundreds of man-years
- Hude code: the graph of functions calls (their names, arguments, and arrows) was several dozen pages long

Toward five-dimensional core-collapse supernova simulations

C Y Cardall^{1,2}, A O Razoumov^{1,2,3}, E Endeve^{1,2,3}, E J Lentz^{1,2,3}, and A Mezzacappa¹

¹ Physics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6354, USA

² Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996-1200, USA

³ Joint Institute for Heavy Ion Research, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6374, USA

Abstract. The computational difficulty of six-dimensional neutrino radiation hydrodynamics has spawned a variety of approximations, provoking a long history of uncertainty in the core-collapse supernova explosion mechanism. Under the auspices of the Terrascale Supernova Initiative, we are honoring the physical complexity of supernovae by meeting the computational challenge head-on, undertaking the development of a new adaptive mesh refinement code for self-gravitating, six-dimensional neutrino radiation magnetohydrodynamics. This code—called *GenASiS*, for *General Astrophysical Simulation System*—is designed for modularity and extensibility of the physics. Presently in use or under development are capabilities for Newtonian self-gravity, Newtonian and special relativistic magnetohydrodynamics (with ‘realistic’ equation of state), and special relativistic energy- and angle-dependent neutrino transport—including full treatment of the energy and angle dependence of scattering and pair interactions.

First side project: 2D semi-analytic models of γ -ray bursts

- Initially developed as a toy test problem for GenASiS, took a life of its own
- Several astrophysics scenarios: core collapse with rotation, merger of two neutron stars, other mergers
- In all cases formation of a rotationally supported, short-lived, very dense disk
- Static hydro
- Full neutrino physics (relying on experimentally measured coefficients \Rightarrow no analytic solution)
- Models were built as a function of 2 parameters: total disk mass and the accretion rate

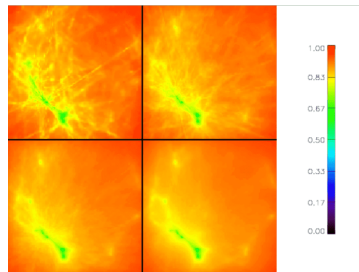
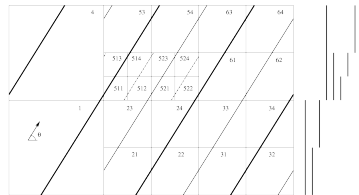
Second side project: fully-threaded transport engine (FTTE)

2005-2006 full solution to the standalone RTE, focusing on performance

- Two independent solvers: “diffuse” (continuous sources) and point-source – both implemented in object-oriented F90

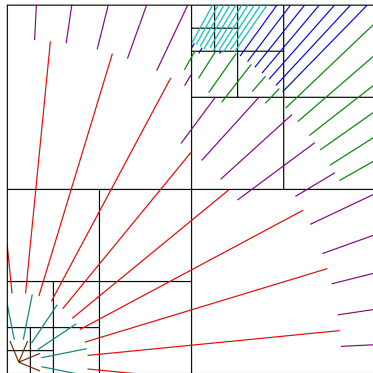
(1) Diffuse solver:

- 3D multi-resolution Cartesian mesh, cell-based AMR, long characteristics starting from the domain boundary and going recursively into higher-resolution cells
- all geometry pre-computed ahead of time, once per angle per 2D layer per resolution level
- all ray elements linked via F90 pointers from its host cell, and vice versa
- during actual transfer follow the interconnected data structures of cells and ray segments precomputed for a particular $(\theta, \phi) \Rightarrow$ fully “threaded”
- zero angular diffusion, HEALPix for angular discretization, fully conservative
- state-of-the-art implementation: benchmarked on scattering in stellar atmospheres, benchmarked against Intel’s ray tracing packages (on much simplified physics) \Rightarrow very competitive performance



(2) Point-source solver:

- uses the same multi-resolution Cartesian mesh
- rays start from points, each splitting hierarchically into four rays as a function of distance and local grid resolution, to satisfy the *min number of ray segments per cell*
- HEALPix for angular discretization, fully conservative
- sources grouped into hierarchical trees \Rightarrow can scale up to tens of thousands of sources on a single CPU
- parallelization part is difficult, as it depends on the underlying problem: standalone RT with a very large grid and a few sources, very large number of sources, coupled CFD + RT



-
- Used both in a series of papers with Jesper Sommer-Larsen and Peter Laursen (Copenhagen)
 - f_{esc} of ionizing photons in early galaxies
 - Ly α radiative transport
 - Vastly better than any Monte Carlo RT (faster, more accurate)
 - Also forked it to do [my own 3D visualization](#) (all coded in F90)

- Numerical 3D radiative transfer is largely solved ... but the solution needs to be tailored to each specific problem
- F90 implementation (2005-2006) of the “diffuse” part is at <https://github.com/razoumov/radiativeTransfer.git>
 - assumes very specific memory storage format for nested cells \Rightarrow likely cannot be used directly in someone else’s code
- General 3D RHD is still an unsolved problem
 1. discretized problem size: likely 6D (and not 5D) for coupled equations
 2. source/sink “slider”
 3. all those pesky $O(v/c)$ terms
 4. parallelization

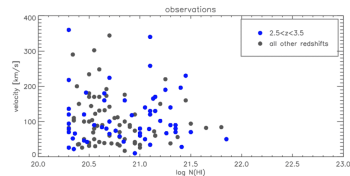
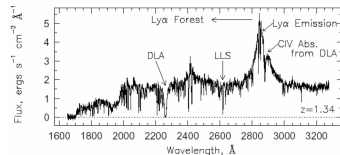
3rd postdoc: free to work on any project

2006-2009 at the ICA at Saint Mary's University in Halifax

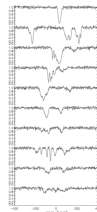
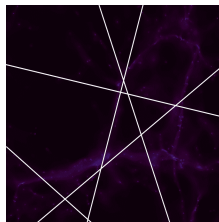
1. Radiative transport in early galaxies with J. Sommer-Larsen and P. Laursen
2. Damped Ly α absorbers (DLAs): trying to explain large observed gas velocity dispersion
3. Galactic disks with star formation and feedback (related to the previous problem)

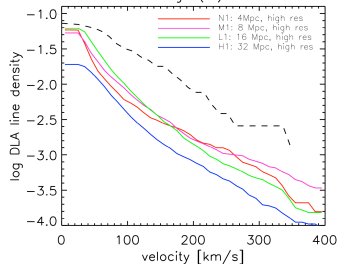
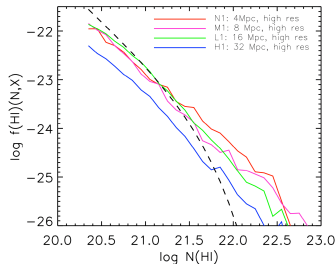
DLAs

- Ly α forest: $N(\text{HI}) < 10^{17} \text{cm}^{-2}$, $\delta\rho/\rho \sim 10$
- Lyman-limit systems: $10^{17} \text{cm}^{-2} < N(\text{HI}) < 2 \times 10^{20} \text{cm}^{-2}$, $\delta\rho/\rho \sim 100$
- Damped Ly α absorbers (DLAs): $N(\text{HI}) > 2 \times 10^{20} \text{cm}^{-2}$, $\delta\rho/\rho \gg 100$
 - probe neutral interstellar medium in forming proto-galaxies
 - dominant reservoir of neutral gas at high redshifts



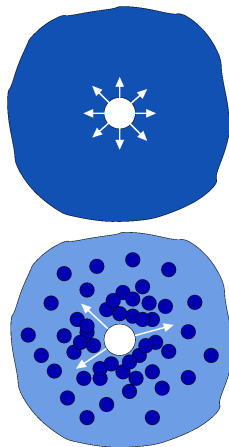
1. run a big simulation
2. draw $\sim 10^6$ random lines of sight
3. calculate line profiles in the velocity space
4. add $S/N=20$ for each 1 km/s pixel
5. line widths from 90% optical depth
6. multiple components within 400 km/s considered a single line





Models fail to explain large observed gas velocity dispersion ...

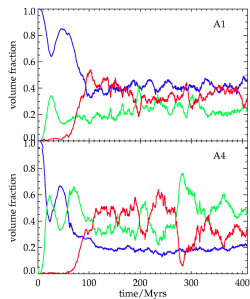
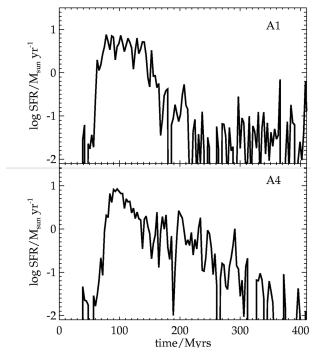
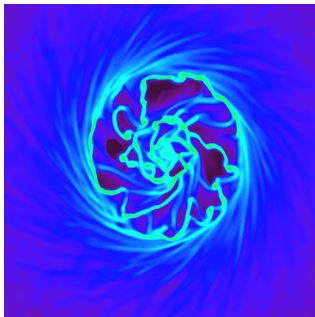
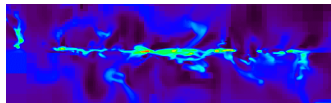
Injection of $1.8 \times 10^{50} \text{ erg/yr} / 10^{12} M_{\odot}$ into cloud kinetic energy would provide the right velocity dispersion



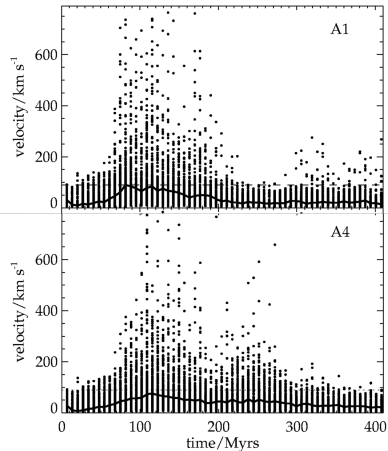
Problem: at low numerical resolution energy spread over too large a mass \Rightarrow temperature too low, cooling probably overestimated

How to grow hot bubbles in the interstellar medium

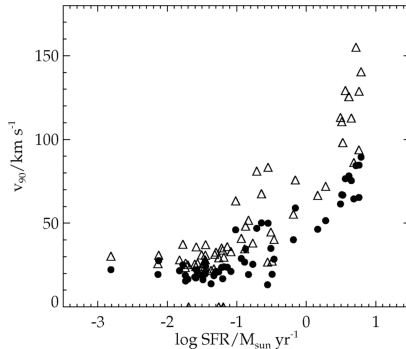
1. Heating must dominate over cooling
2. In hot regions pressure must overcome self-gravity
3. Single SN explosion must heat gas to $\sim 10^{7.5}$ K
4. Need high density contrast to preserve some of ongoing star formation
5. Need to use a sufficiently high density star formation threshold to decouple SF rates from the exact prescription ($n_H \geq 6500 \text{ cm}^{-3}$)



Volume fraction of **cold**, **warm**, **hot** phases in the galactic midplane



Most HI absorption comes from within
 $\sim 1\text{kpc}$ above/below the disk



Good velocity dispersion, but somewhat inconsistent
 with very low observed star formation rates in DLAs

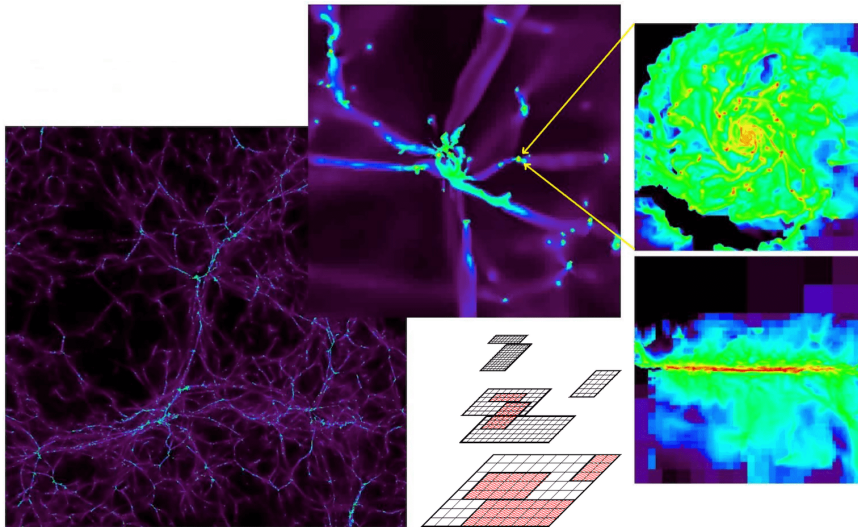
Range of scales

Cosmological simulations

- 50 pc spatial resolution
⇒ no reasonable outflows
- subgrid multiphase models: good for self-regulation of SF/feedback but do not separate phases dynamically

ISM models in isolated galaxies

- what spatial resolution is needed to resolve multiphase ISM in which thermal feedback would launch realistic winds – probably 10 pc or better
- need to resolve feedback from individual SNe



Dynamic range 10 Mpc - 10 pc

2009-2014

- HPC Consultant with SHARCNET, based at UOIT (now Ontario Tech University) near Toronto
- Working on programming projects, HPC problem tickets, general support in multiple domains, and training in HPC
- Organized biweekly in-person scientific computing seminars in the Faculty of Science

2014-present

- Working for WestGrid / Compute Canada / SFU – really the same evolving position
 - initially hired as a visualization specialist, quickly expanded to cover broader training and support
- Now with the Research Computing Group at SFU
 1. leading a 2-person training team at SFU (Marie-Hélène Burle and myself), providing research computing (RC) and HPC training and support in Western Canada
 2. responsible for sci-vis support across the country, leading the National Visualization Team since 2014
- Teaching ~90 events per year
 - biweekly webinars (since 2015)
 - weekly online courses (since 2023)
 - week-long in-person summer/winter/etc schools (since 2017)
 - various national series and invited schools, local and one-off workshops, bootcamps, hackathons, etc.
- All our training is free to academic researchers in Canada
- Teaching ~20 full-day courses in RC and HPC
 - sliced and offered in different formats
 - all levels from beginner's command line to large-scale parallel programming and niche topics
 - constantly developing new materials
 - limited bandwidth \Rightarrow do not teach domain-specific computing, typically cycling through courses throughout an academic year, always struggling between depth and the number of topics

Courses

Each title amounts to ~1 day of materials; more details at <https://training.westdri.ca>

Remote computing basics

- Bash command line
- Introduction to HPC

Programming tools

- Basics of Python
- Basics of R
- Introductory Julia
- Scientific Python

Parallel coding

- Parallel programming in Chapel
- Parallel computing in Julia
- HPC Python
- Speeding up computations with parallel R
(used to teach MPI/OpenMP/GPUs, but no bandwidth)

Virtualization

- Intro to the Alliance cloud and VMs
- Intro to Apptainer containers

Machine learning

- Deep learning with PyTorch
- Deep learning with JAX and Flax

Scientific visualization

- 3D sci-vis with ParaView
- 3D sci-vis with VisIt
- 3D visualization for the humanities
- Remote and large-scale rendering
- Many other shorter visualization topics: in-situ vis, topological data analysis, photorealistic rendering, custom ParaView filters and plugins, many 1D/2D plotting packages, 3D multi-resolution vis with YT, etc.

RDM topics

- Version control with Git
- Large data version control with Datalad, git-annex, DVC
- Managing files and formats: scientific formats and data libraries, parallel I/O, overlays, etc.

- Subscribe to our weekly emails (Sep-May)
<https://bit.ly/rcweeklylist>
- Send us topic suggestions
- Doing this as part of RC/HPC training across the Alliance Federation

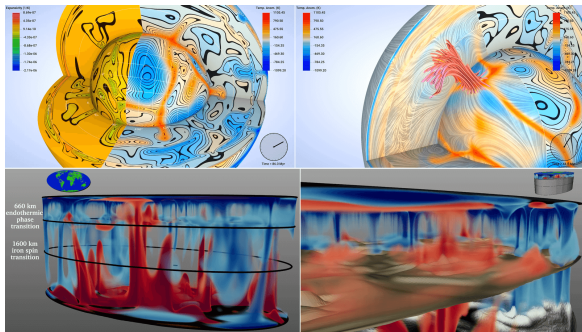
Biweekly webinars

- Focusing on more advanced, well-defined, shorter topics typically not covered in our regular training
 - we use these as test vehicles for new training topics
 - valuable service to researchers, since most have no knowledge of these tools / techniques
 - often covering topics that do not have good documentation \Rightarrow quite research heavy, often requiring hundreds of hours of preparation
 - sometimes quite a scary experience, as these webinars can attract world experts in niche topics
- For upcoming webinars and registration links see <https://training.westdri.ca/blog>
 - fall 2024 scheduled will be published by the end of August
- \sim 150 webinars archived at <https://training.westdri.ca>, both **chronologically** and by **topic**
- Currently delivered by a team of two \Rightarrow looking for collaborations

Visualization support and training

Details at <https://ccvis.netlify.app>

- Visualization webinars is just one aspect
<https://bit.ly/vispages>
- National Visualization Team since 2014: 5-6 HPC analysts interested in sci-vis
- Vis. queue in the national ticket system
- Centered around ParaView and VTK
 - modern standard for 3D sci-vis
 - open-source, general-purpose, multi-platform
 - scalable to tens of thousands of cores, TBs of data
 - scriptable, remote client-server and batch rendering, in-situ (Catalyst), Cinema science
- Very familiar with many other sci-vis tools as well (VisIt, YT, VMD, ...)
- National visualization contests since 2016 <https://ccvis.netlify.app/contests>
 - provide 1-2 datasets, give some tasks
 - in 2021 chaired the international IEEE Sci-Vis Contest
 - zero budget for prizes, no comms support of any kind, do everything ourselves



Summary

- Shockingly, **computational astrophysics** was not taught properly at all institutions I worked, even places like the ICA@SMU
 - pretty much the same can be said about teaching **numerical methods** to physicists
 - would be very happy to develop / teach beginner's courses
- Writing simulation code is easy; making sure it works as projected takes orders of magnitude longer
- If you publish (numerical simulations), your problem is probably too simple
- Standalone 3D radiative transfer is a solved problem: get in touch
alex.razoumov@westdri.ca
- Coupled RHD remains a challenge: again, get in touch