AI in the Sciences and Engineering HS 2025: Lecture 1

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Seminar for Applied Mathematics (SAM), D-MATH (and),
ETH AI Center (and) Swiss National AI Institute (SNAI) ,
ETH Zürich, Switzerland.

Practical Information

- Lectures in MLH44: Thursday 8.15am – 10 am.
- Live Broadcast on Zoom + Recordings.
- Recordings will be available on Course Moodle page.
- Organizers:
  - Bogdan Raonic
  - Shizheng Wen
- No Exams !!
- Performance Assessment: Project Work[1]
- Tentative date of release of Projects: 10.12.25
- Tentative date of Project Submission: 20.1.25
- Course Material:
  - Lecture Recordings + Slides
  - All Material is based on research $<$ 4 years.

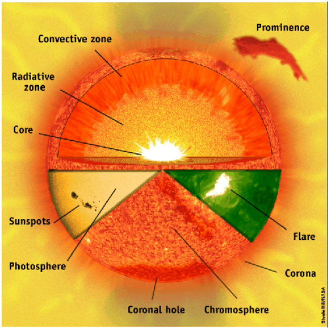
[1] NO questions about projects during lectures and tutorials !!!

Course Contents

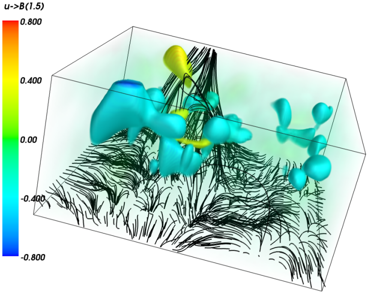
- Present latest applications of AI in Science and Engineering.
- Split into 2 parts.
- Part I: AI in Physics and Engineering.
- Taught by SM
- Bulk of the course.
- Part II: AI in Chemistry and Biology.
- Taught by David Graber
- Tutorials supplement course content with Programming demos.

What happens in Science and Engineering ?

Physics: What heats the Solar Corona to 10^6 degrees ?

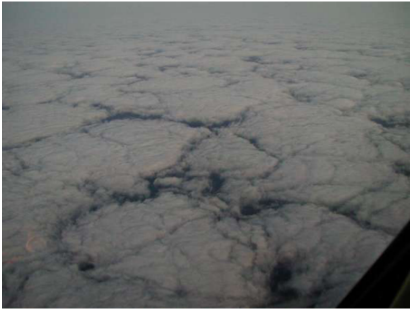


Sun

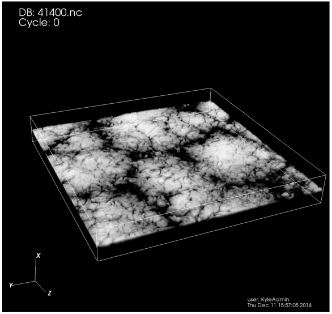


Solar Waves

Climate Science: How do Stratocumulus Clouds affect Climate Change?

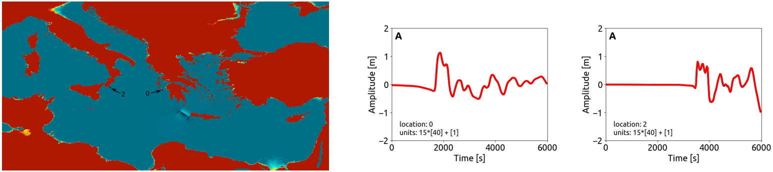


Measurement

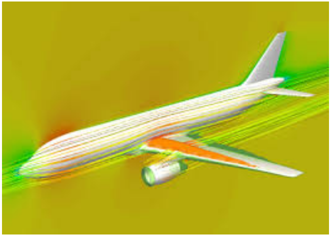


Simulation

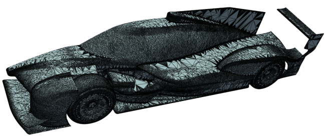
Geophysics: Tsunami Early Warning System

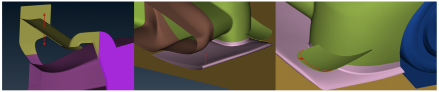


Engineering: How to design a more Fuel efficient Aircraft ?

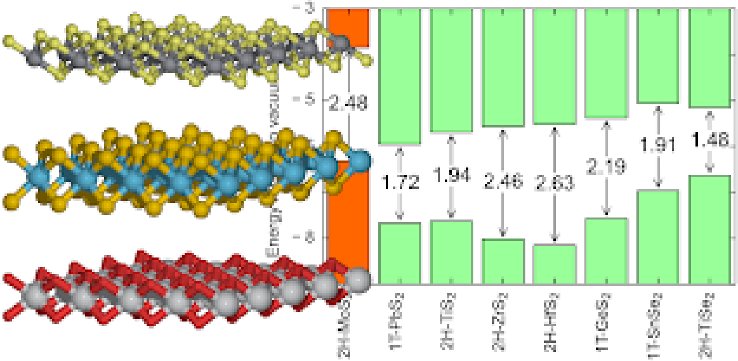


Engineering: or a faster Race Car ?

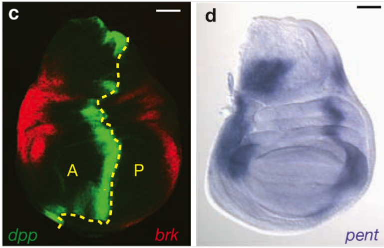




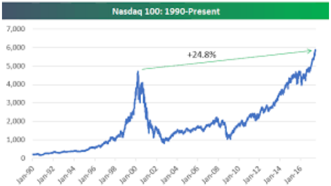
Chemistry: What is the electronic structure of a novel nanomaterial ?

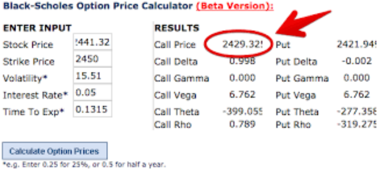


Biology: Why is a fly wing pattern robust to growth ?



Finance: What is the right price for a stock option ?





How are these problems solved currently ?

Step 1: Mathematical Modeling

The general paradigm is : given a blueprint, to find the corresponding recipe. Much of the activity of science is an application of that paradigm : given the description of some natural phenomena, to find the differential equations for processes that will produce the phenomena.

- A prize quote from Herbert Simon (Nobel prize in Economics, 1978)
- Given a scientific problem, find a Partial Differential Equation (PDE) describing it

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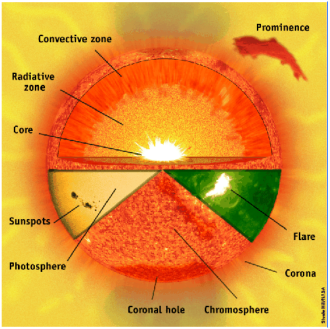

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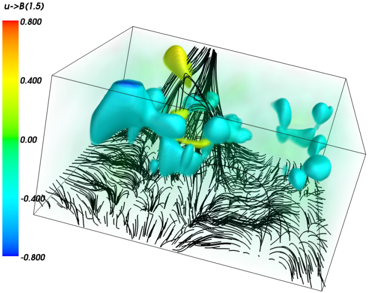

Solar Waves

MHD equations

- Conservation of mass, momentum, energy and Magnetic field.

$$
\begin{aligned}
\rho_t + \mathrm{div}(\rho \mathrm{u}) &= 0, \\
(\rho \mathrm{u})_t + \mathrm{div}(\rho \mathrm{u} \otimes \mathrm{u} + (p + \frac{1}{2}|\mathrm{B}|^2)I - \mathrm{B} \otimes \mathrm{B}) &= \mathcal{D}_{\mathrm{u}} + \mathcal{F}, \\
E_t + \mathrm{div}((E + p + \frac{1}{2}|\mathrm{B}|^2)\mathrm{u} - (\mathrm{u} \cdot \mathrm{B})\mathrm{B}) &= \mathcal{D}_E, \\
\mathrm{B}_t + \mathrm{div}(\mathrm{u} \otimes \mathrm{B} - \mathrm{B} \otimes \mathrm{u}) &= \mathcal{D}_{\mathrm{B}}, \\
\mathrm{div}(\mathrm{B}) &= 0.
\end{aligned}
$$

- Together with equation of state

$$
E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho|\mathrm{u}|^2 + \frac{1}{2}|\mathrm{B}|^2,
$$

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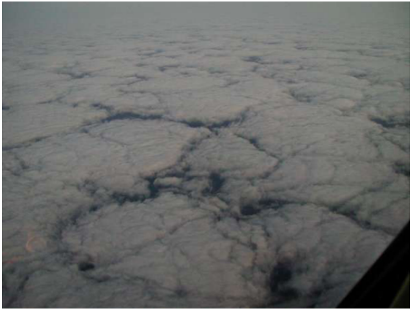

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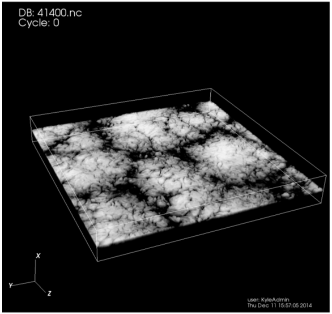


Simulation

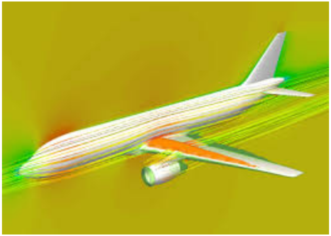
Equations of motion.

- Anelastic Euler equations for momentum + Scalar transport:

$$
\begin{aligned}
(\bar{\rho} u)_t + \mathrm{div}(\bar{\rho} u \otimes u) + \nabla p &= S_b + S_{ev} + S_T^u \\
\mathrm{div}(\bar{\rho} u) &= 0, \\
(\bar{\rho} s)_t + \mathrm{div}(\bar{\rho} u s) &= S_T^s + S_{ed}^s \\
(\bar{\rho} q)_t + \mathrm{div}(\bar{\rho} u q) &= S_T^q + S_{ed}^q
\end{aligned}
$$

- Specified density $\bar{\rho}$, velocity u, specific entropy s and water specific humidity q.
- Bouyancy S_b.
- Complicated coupled Thermodynamic source terms $S_T^{u,s,q}$
- Add variables such as Precipiation, Snow etc.

Engineering: How to design a more Fuel efficient Aircraft ?



Governing Equations

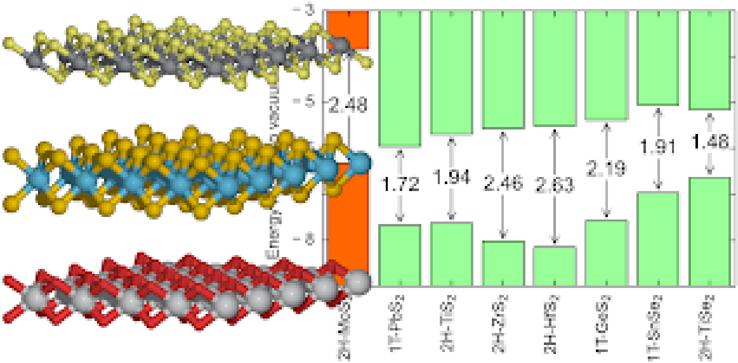
- Compressible Euler equations:

$$
\begin{aligned}
\rho_t + \mathrm{div}(\rho \mathrm{u}) &= 0, \\
(\rho \mathrm{u})_t + \mathrm{div}\left(\rho \mathrm{u} \otimes \mathrm{u} + p\mathrm{I}\right) &= 0, \\
E_t + \mathrm{div}\left((E + p)\mathrm{u}\right) &= 0.
\end{aligned}
$$

- With Equation of state:

$$
p = \gamma - 1 \left(E - \frac{1}{2}\rho|\mathrm{u}|^2 \right)
$$

Chemistry: What is the structure of a novel nanomaterial ?



PDEs for Electronic Structure

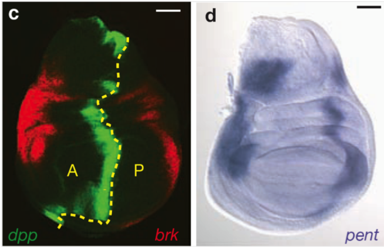
- Some version of Schrödinger's Equation
- Time-dependent version for Wave function $\Psi \in H$:

$$\iota h \frac{d\Psi}{dt} = H\Psi(t)$$

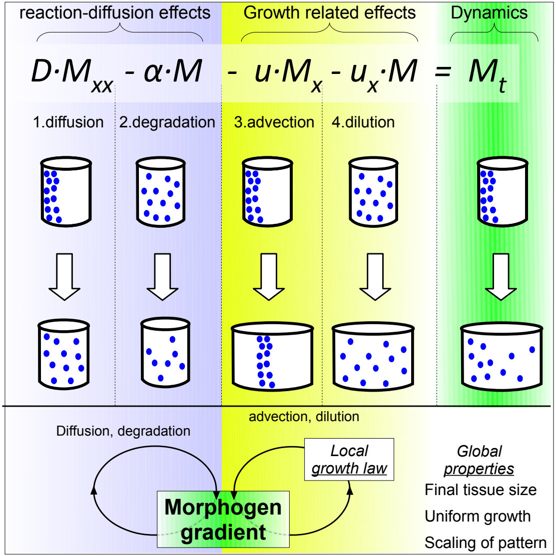
- with Many-body Quantum Hamiltonian:

$$H := \left(-\sum_{i=1}^{N} \frac{h^2}{2m_i} \Delta_{r_i} + \sum_{i=1}^{N} V_{ext}(r_i) + \sum_{1 \leq i,j \leq N} W_{ij}(r_i, r_j) \right)$$

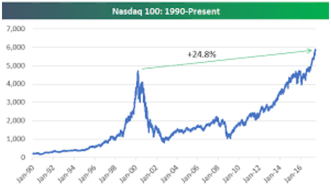
Biology: Why is a fly wing pattern robust to growth ?



PDEs for Morphogenesis: Reaction-Diffusion Equations



Finance: What is the right price for a stock option ?



Black-Scholes Option Price Calculator (Beta Version):

ENTER INPUT		RESULTS			
Stock Price	:441.32	Call Price	2429.32!	Put	2421.94!
Strike Price	2450	Call Delta	0.998	Put Delta	-0.002
Volatility*	15.51	Call Gamma	0.000	Put Gamma	0.000
Interest Rate*	0.05	Call Vega	6.762	Put Vega	6.762
Time To Exp*	0.1315	Call Theta	-399.05!	Put Theta	-277.358
		Call Rho	0.789	Put Rho	-319.27!

Calculate Option Prices

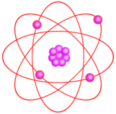
*e.g. Enter 0.25 for 25%, or 0.5 for half a year.

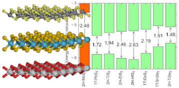
Option pricing PDEs

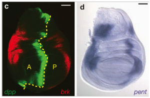
- Variants of Black-Scholes PDEs
- Example: Black-Scholes with Uncorrelated noise:

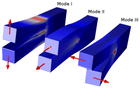
$$u_t = \frac{1}{2}\sum_{i=1}^{d}(\sigma_i x_i)^2 u_{x_i x_i} + \sum_{i=1}^{d} \mu x_i u_{x_i}$$

Partial Differential Equations (PDEs): Language of Nature

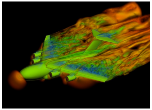


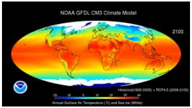


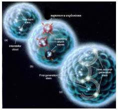


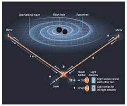


Schrödinger — Kohn-Sham — Reaction-Diffusion — Phase-Field









Euler — Navier-Stokes ++ — MHD++ — Einstein

- Immense diversity of Physical processes
- Very wide range of spatio-temporal scales

What are PDEs ?

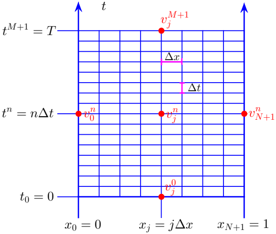
- Generic form of PDEs:

$$\mathcal{F}\left(x, t, u, \nabla u, u_t, u_{tt}, \nabla^2 u, \ldots, \ldots\right) = 0.$$

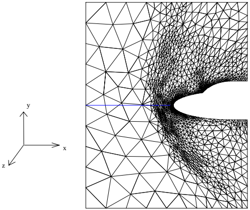
- Here $u : D \times (0, T) \mapsto \mathbb{R}^m$ for $D \subset \mathbb{R}^d$

Numerical Methods

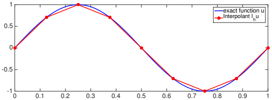
- Not possible to find solution formulas for PDEs.



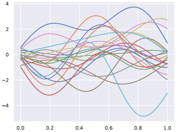
Finite Difference



Finite Volume

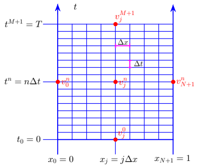


Finite Element



Spectral Method

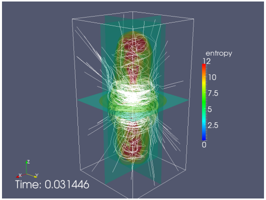
Finite Difference Schemes (FDS) for the Heat Equation



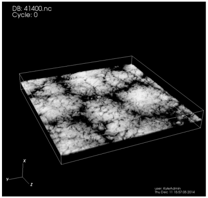
- Heat equation is $u_t = u_{xx}$, Initial conditions: $u(x,0) = \bar{u}(x)$, Boundary conditions: $u(0,t) = u(1,t) = 0$.
- $u_t(x_j, t^n) \approx \frac{v_j^{n+1} - v_j^n}{\Delta t}$, $u_{xx} \approx \frac{v_{j+1}^n - 2v_j^n + v_{j-1}^n}{\Delta x^2}$
- Finite Difference Scheme:

$$v_j^{n+1} = (1 - 2\lambda)v_j^n + \lambda(v_{j-1}^n + v_{j+1}^n), \quad \lambda = \frac{\Delta t}{\Delta x^2}$$

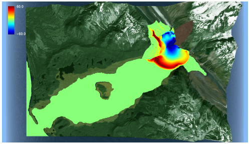
Numerical Methods are very Successful



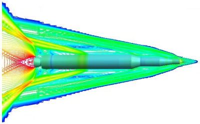
Supernovas



Clouds



Tsunamis



Rockets

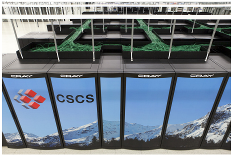
Wheres the Caveat ?

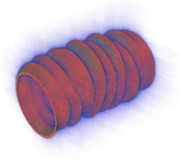
- For stability (CFL): $\Delta t \sim \Delta x^2$.
- Error: $E = E_{\Delta x} \sim \Delta x^2$
- $\#$ (meshpoints) $\sim \Delta x^{-d}$, $\#$ (timesteps) $\sim \Delta t^{-1} \approx \Delta x^{-2}$,
- Compute: $\mathcal{C} \sim \frac{1}{\Delta x^{d+2}}$
- Computational Complexity: $\mathcal{C} \sim \left(\frac{1}{E}\right)^{\frac{d+2}{2}}$
- Compute grows exponentially with dimension

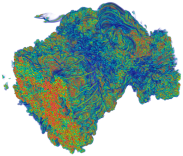
PDEs in high dimensions: $d \geq 4$

- Boltzmann Equation ($d = 7$)
- Radiative Transfer Equation ($d \geq 5$)
- Computational Finance: Black-Scholes ($d >> 1$)
- Computatational Chemistry: Schrödinger ($d >> 1$).

Issues with Numerical Methods even in low Dimensions

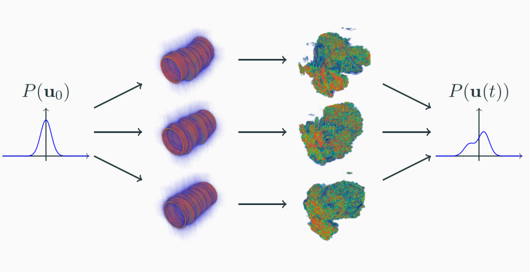






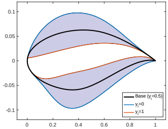
- Computational Cost !!: PDE solvers can be very expensive.
- Simulation of Navier-Stokes at 1024^3:
  - With Azeban on Piz Daint.
  - Single Run: 94 GPU hours.
  - Single Run: 4512 CPU hours
- Significant HR Cost !!

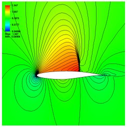
Many-Query Problems I: UQ

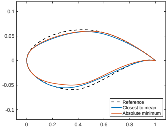


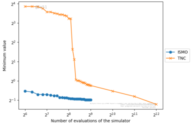
- UQ often based on Monte Carlo Random sampling.
- Requires multiple calls to PDE solvers.
  - With Azeban on Piz Daint.
  - Single Sample: 94 GPU hours.
  - Ensemble simulation: 96256 node hours

Many-Query Problems II: PDE Constrained Optimization





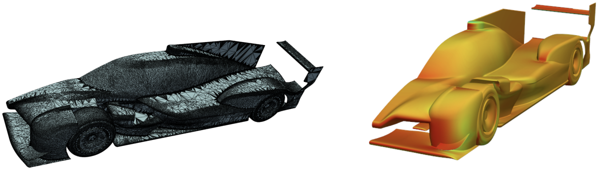




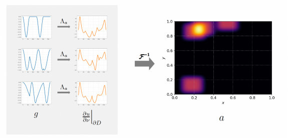
- Airfoil Shape Optimization.
- Parametrized Airfoils with Hicks-Henne shape functions.
- Optimization with Gradient descent.
- At each step: Forward solution of Compressible Euler Eqns.
- Adjoint solve to compute gradients.
- Forward solve with NUWTUN: 10^2 secs.
- Adjoint solve: 10^2 secs.
- Total computational time: 228 hrs !!!

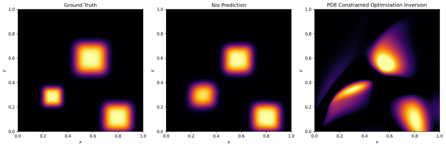
An Industrial Example ?

- Flow past Race car simulation requires 500 node hours per shape !!



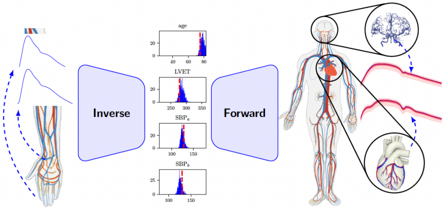
Many-Query Problems III: PDE Inverse Problems





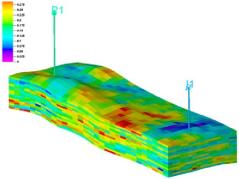
- Inclusion detection by Wave Scattering
- Wave motion modeled by Helmholtz Eqns.
- Inverse map: Dirichlet-to-Neumann operator $\mapsto$ Coefficient
- Solve using gradient descent.
- Total run time for $\mathcal{O}(10^3)$ evals: 8.5 hrs.
- Total Error: 11.2%

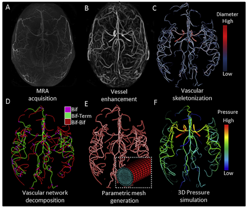
Many-Query Problems IV: Bayesian Inversion

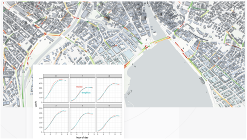


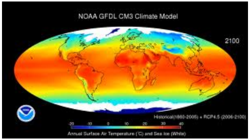
- Parameter inference for Human Cardiovascular System
- Uses MCMC for Bayesian Inversion.
- Each forward solve for Conservation Laws is 2 min.
- Needs $\mathcal{O}(10^4)$ forward solves.
- Total runtime: 330 hrs.

Unknown or Incomplete Physics





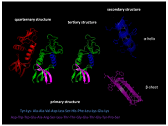


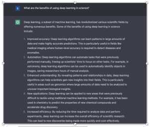


- Missing Physics not just undetermined parameters.
- Manifestation of Sim2Real gap.
- Holds True for most real-world applications.
- Still have Data for underlying operators

Key Aim of this Course: *Learn Physics modeled by PDEs from data*

The age of AI




- 3 Pillars of Success !!
- Exponentially more Compute aka GPUs :-)
- Huge Data
- Deep Neural Networks