Title: Special Topics in Astrophysics - Numerical Hydrodynamics - Lecture 4

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CUBE – Towards an Optimal Scaling of Cosmological N-body Simulations

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***Abstract*—N-body simulations are essential tools in physical cosmology to understand the large-scale structure (LSS) formation of the universe. Large-scale simulations with high resolution are important for exploring the substructure of universe and for determining fundamental physical parameters like neutrino mass. However, traditional particle-mesh (PM) based algorithms use considerable amounts of memory, which limits the scalability of simulations. Therefore, we designed a two-level PM algorithm CUBE towards optimal performance in memory consumption reduction. By using the *fixed-point compression* technique, CUBE reduces the memory consumption per N-body particle to only 6 bytes, an order of magnitude lower than the traditional PM-based algorithms. We scaled CUBE to 512 nodes (20,480 cores) on an Intel Cascade Lake based supercomputer with $\simeq 95\%$ weak-scaling efficiency. This scaling test was performed in Cosmo-π – a cosmological LSS simulation using $\simeq 4.4$ trillion particles, tracing the evolution of the universe over $\simeq 13.7$ billion years. To our knowledge, Cosmo-π is the largest completed cosmological N-body simulation. We believe CUBE has a huge potential to scale on exascale supercomputers for larger simulations.**

***Index Terms*—N-body, particle-mesh method, large-scale sim-**

A direct-summation algorithm is unaffordable for a large N because the computational complexity of such a pairwise force (PP force) calculation is $O(N^2)$. Many algorithms have been designed to reduce the complexity to $O(N \log N)$, such as the particle-mesh (PM) or tree methods, or even $O(N)$, such as the fast multipole method. Fortunately, cosmological N-body simulations rarely require accurate trajectories of individual particles, but rather just correct statistical distributions. In this scenario, the PM-based algorithms usually meet the accuracy requirements and have a potential to simulate with a very large N.

However, achieving the largest N with the PM-based algorithms is typically bound by memory capacity, instead of computing capacity. For example, TianNu [2], one of the world's largest N-body simulations, used the P^{3}M algorithm [3] to complete an $N \simeq 3 \times 10^{12}$ cosmological N-body simulation on the Tianhe-2 supercomputer. The simulation used

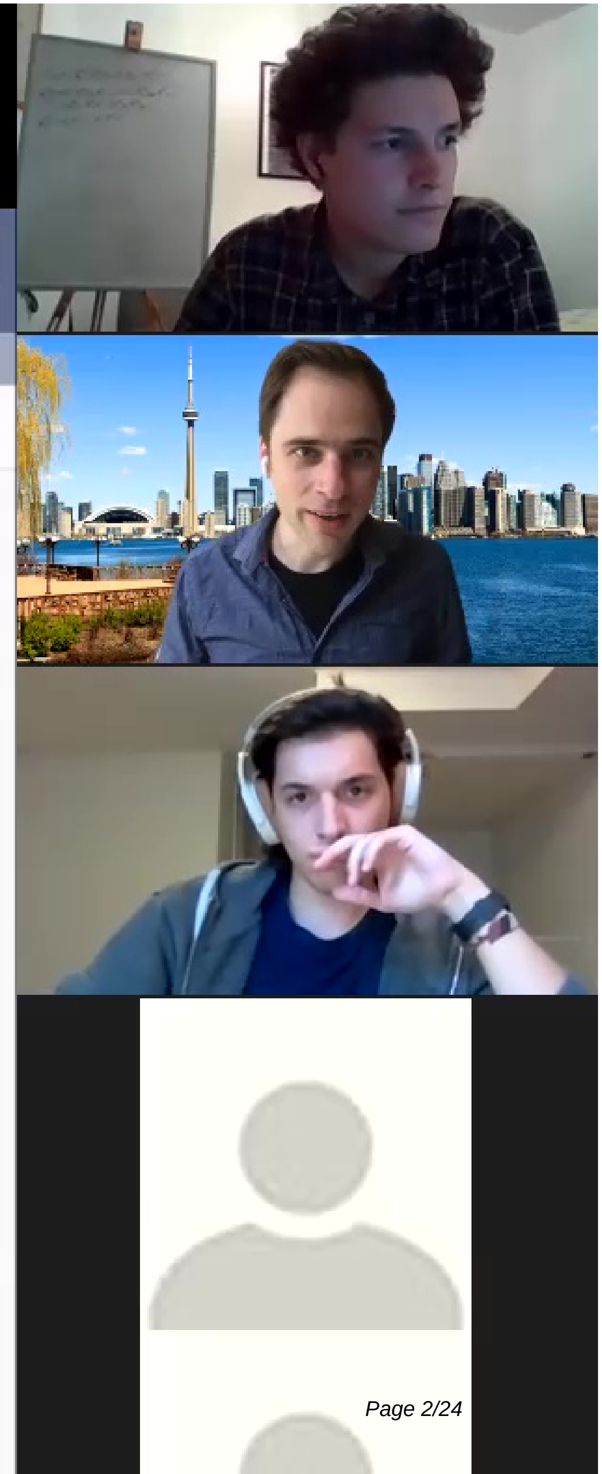

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TABLE II: Comparison of the large-scale cosmological N-body simulations on supercomputers. For each simulation, we summarize the computational scale in CPU cores (c) or GPU cards (g), the problem scale in the particles number (N_p), redshift range (z_i, z_f), box size (L), method used to compute the force, and force resolution (ϵ). To the best of our knowledge, this work is the largest cosmological N-body simulation (4.39 trillion particles).

Simulations	Years	Codes	Supercomputers	Scale	$N_p(\times 10^{12})$	z_i, z_f	L (Gpc/h)	Force	ϵ (kpc/h)
Dark Sky [15]	2014	2HOT	Titan	12,288g [1]	1.074	93, 0	8	Tree	36.8
ν^2GC [16]	2015	GreeM[3]	K Computer	131,072c	0.55	127, 0	1.12	TreePM	4.27
Q Continuum [17]	2015	HACC	Titan	16,384g [1]	0.55	200, 0	0.923	P^3M	2
TianNu [2]	2017	CUBEP^{3}M	Tianhe-2	331,776c	2.97	5, 0	1.2	PM-PM-PP	13
Euclid Flagship [18]	2017	PKDGRAV3	Piz Daint	>4,000g [1]	2.0	49, 0	3	FMM	4.8
Outer Rim [19]	2019	HACC	MIRA	524,288c	1.074	200, 0	3	TreePM	2.84
Cosmo-π (This work)	2019	CUBE	π 2.0	20,480c	**4.39**	99, 0	3.2	PM-PM	195

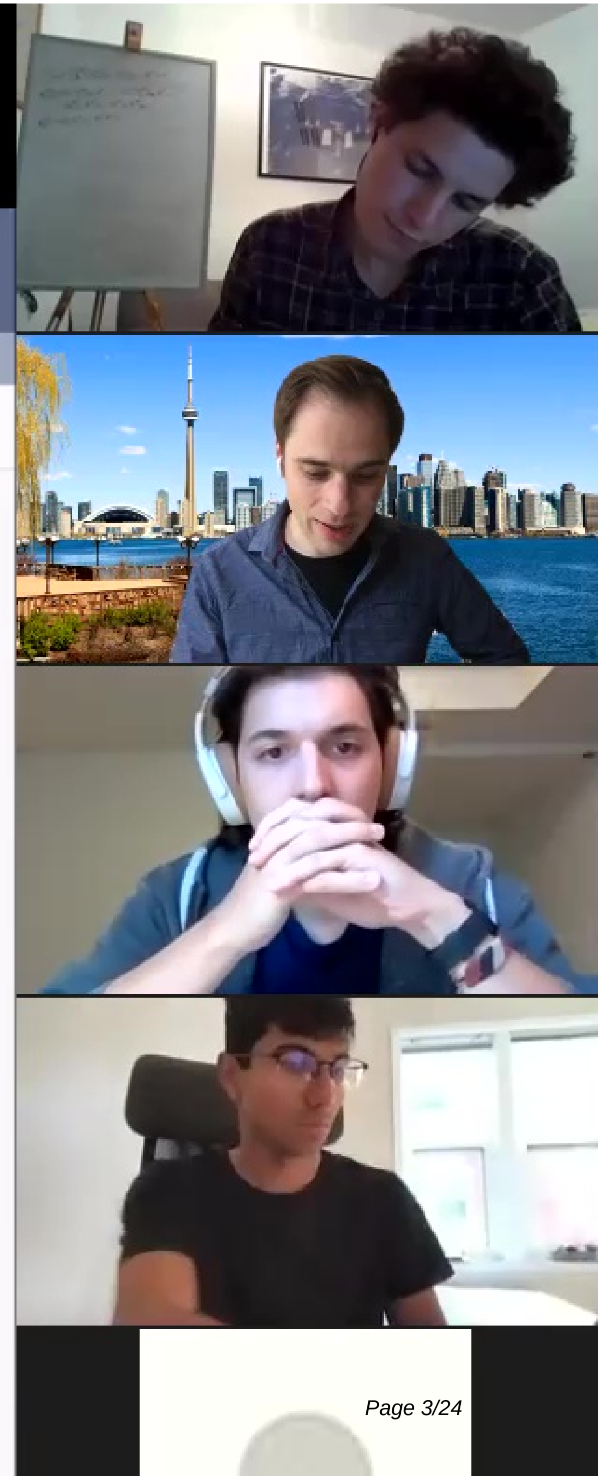
1. These three simulations were carried out using NVIDIA Tesla K20X.

VI. Impact of the Solution

We summarize the impact of the Cosmo-π simulation in three aspects. First, Cosmo-π is, to the best of our knowledge, the largest completed cosmological N-body simulation, evolving 4.39 trillion particles from redshift 99 to 0. Simulations such as Cosmo-π, as well as higher resolution ones using the PP force, will allow for improved LSS statistics and better understanding of halo assembly and substructure.

Second, we believe CUBE has a huge potential for large-scale cosmological simulations. Cosmo-π was able to evolve 4.39 trillion particles using just 20,480 cores, a substantial improvement in N enabled by CUBE's memory consumption optimization. In the next few years, exascale supercomputers

[5] U.-L. Pen, "A Linear Moving Adaptive Particle-Mesh N-Body Algorithm," ApJS, vol. 100, p. 269, Sep. 1995.
[6] H. Merz, U.-L. Pen, and H. Trac, "Towards optimal parallel PM N-body codes: PMFAST," New A, vol. 10, pp. 393–407, Apr. 2005.
[7] S. Rajan, S. Wang, R. Inkol, and A. Joyal, "Efficient approximations for the arctangent function," *IEEE Signal Processing Magazine*, vol. 23, no. 3, pp. 187–198, 2006.
[8] A. Rodriguez, E. Sen, E. Meiri, E. Fomenko, Y. Jin, H. Shen, and Z. Barukh, "Lower numerical precision deep learning inference and training," 2018.
[9] Y. B. Zel'dovich, "Gravitational instability: An approximate theory for large density perturbations," A&A, vol. 5, pp. 84–89, Mar. 1970.
[10] J. D. Emberson, H.-R. Yu, D. Inman, T.-J. Zhang, U.-L. Pen, J. Harnois-Déraps, S. Yuan, H.-Y. Teng, H.-M. Zhu, X. Chen, and Z.-Z. Xing, "Cosmological neutrino simulations at extreme scale," *Research in Astronomy and Astrophysics*, vol. 17, p. 085, Aug. 2017.
[11] D. Blas, J. Lesgourgues, and T. Tram, "The Cosmic Linear Anisotropy



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Thermodynamic equilibrium:

$$\frac{\partial f}{\partial t} = 0, \quad \nabla f = 0, \quad \vec{F} = 0 \quad \Rightarrow \quad \frac{Df}{dt} = 0$$

$$\Rightarrow \left[\frac{\partial f}{\partial t}\right]_{coll} \overset{!}{=} 0$$

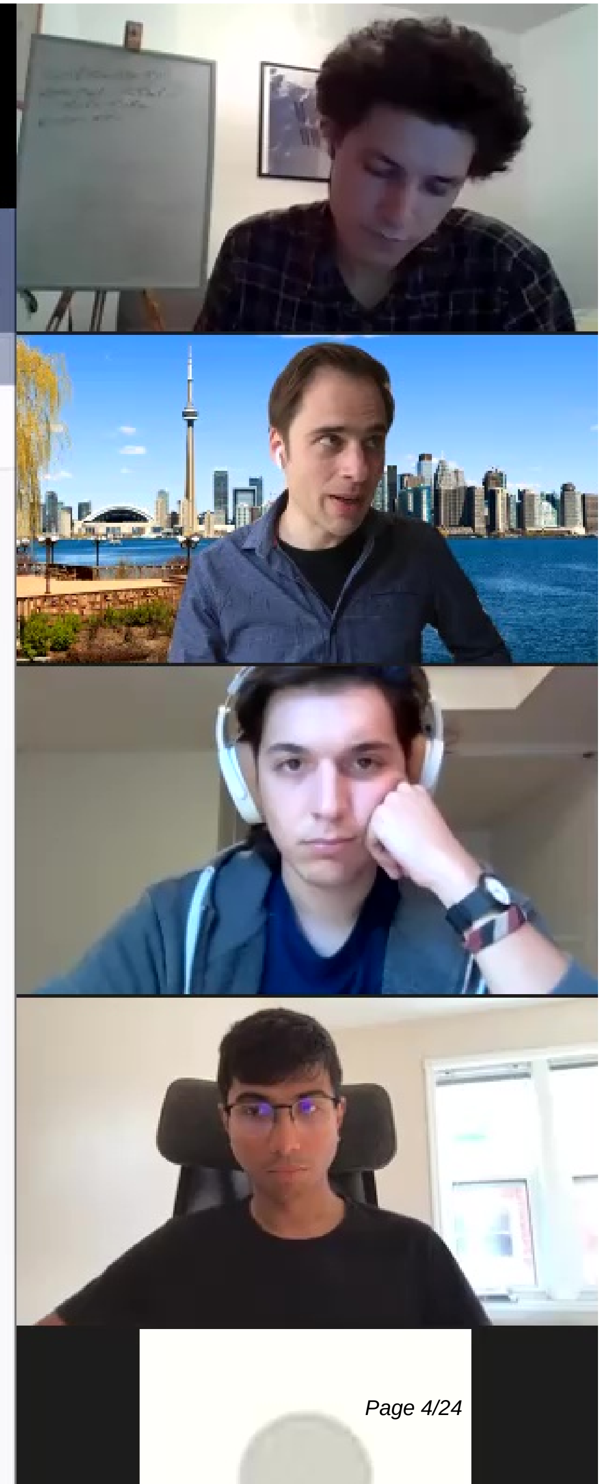
2-particle collisions

$$\Rightarrow \quad f = f_0(\vec{u}) = n\left(\frac{m}{2\pi k_B T}\right)^{3/2} e^{-\frac{m\vec{u}^2}{2k_B T}}$$

T given by $\rho\varepsilon = \frac{3}{2}\frac{k_B}{m}\rho T$

Local thermodynamic equilibrium:

Allow for small gradients in $\rho, \vec{v}, p$ etc.



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distribution
(equilibrium state $t \to \infty$,
$\frac{\partial f}{\partial t} = 0$)

Thermodynamic equilibrium:

$$\frac{\partial f}{\partial t} = 0, \quad \nabla f = 0, \quad \vec{F} = 0 \quad \Rightarrow \frac{Df}{dt} = 0$$

$$\Rightarrow \left[\frac{\partial f}{\partial t}\right]_{coll} \overset{!}{=} 0$$

2-particle collisions $\Rightarrow$ $f = f_0(\vec{u}) = n \left(\frac{m}{2\pi k_B T}\right)^{3/2} e^{-\frac{m \vec{u}^2}{2 k_B T}}$

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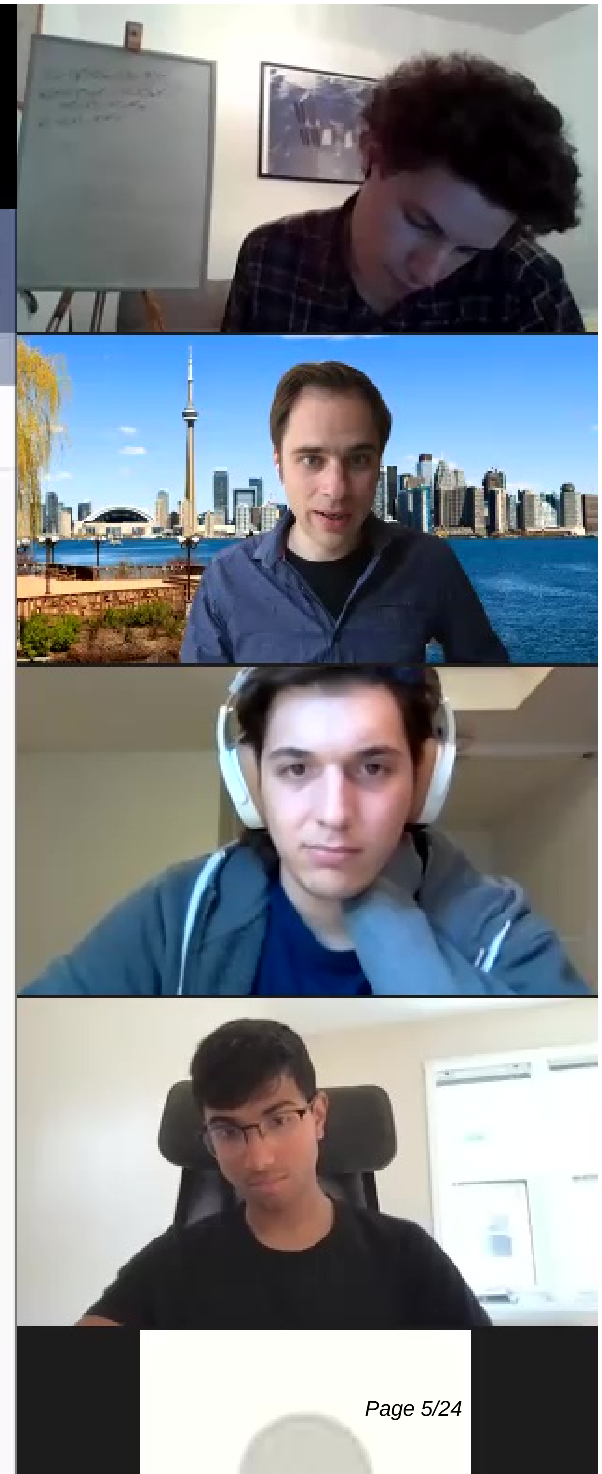

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Thermodynamic equilibrium:

$$\frac{\partial f}{\partial t} = 0, \quad \nabla f = 0, \quad \vec{F} = 0 \quad \Longrightarrow \quad \frac{Df}{dt} = 0$$

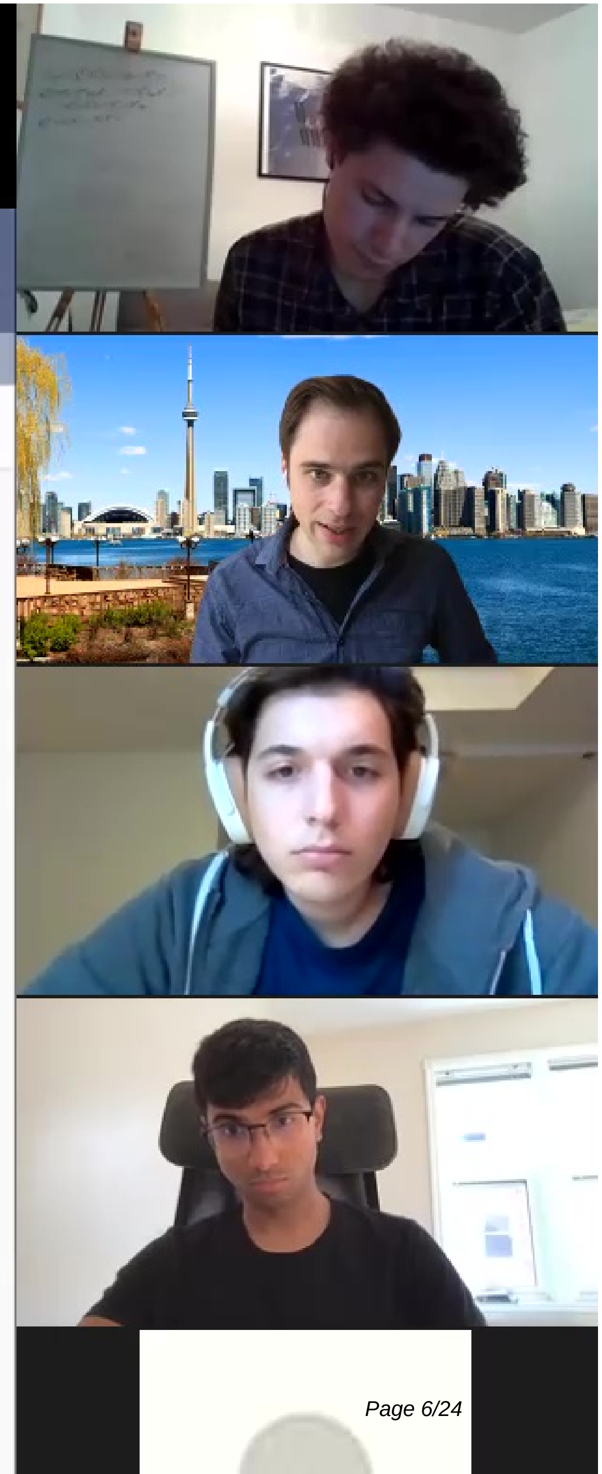
$$\Longrightarrow \left[\frac{\partial f}{\partial t}\right]_{coll} \overset{!}{=} 0$$

2-particle collisions
$$\Longrightarrow f = f_0(\vec{u}) = n\left(\frac{m}{2\pi k_B T}\right)^{3/2} e^{-\frac{m\vec{u}^2}{2k_B T}}$$

T given by $\rho\varepsilon = \frac{3}{2}\frac{k_B}{m}\rho T$

Local thermodynamic equilibrium:

Allow for small gradients in $\rho, \vec{v}, p$ etc.



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3) Validity of continuous medium approximation

(i) $\lambda \ll dx \ll l_{sys}$

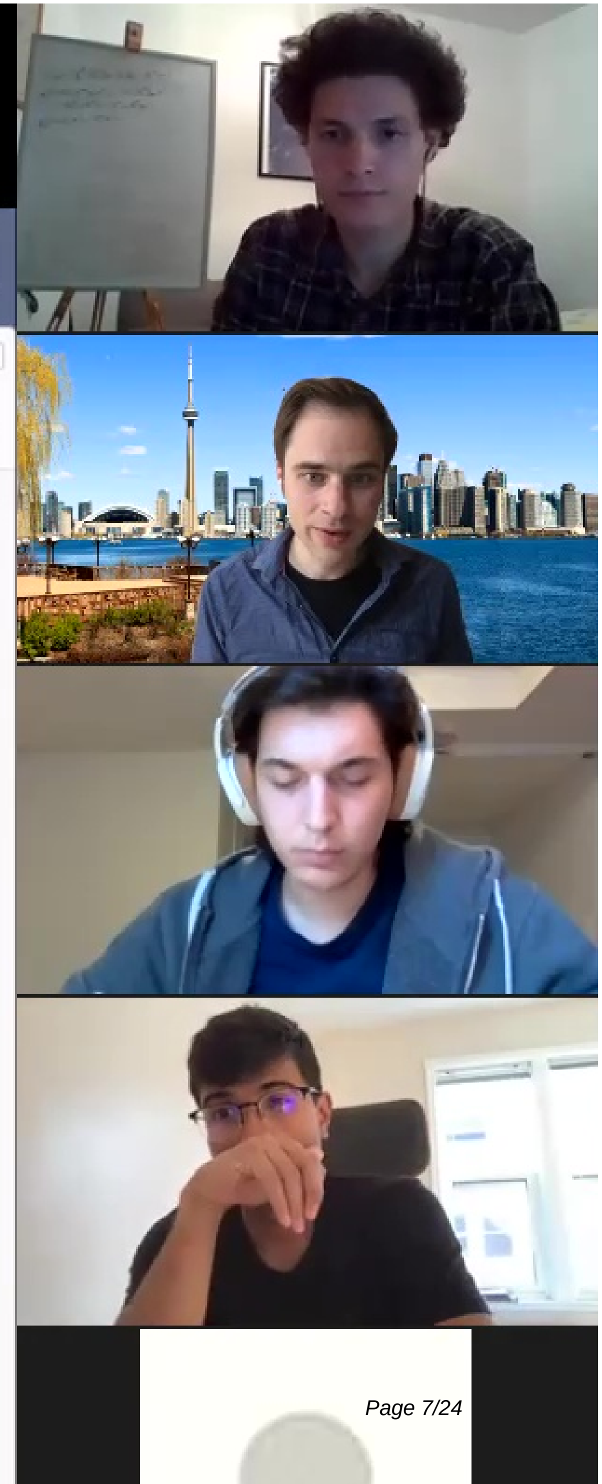
λ: mean free path

dx: finite size of medium elements

l_{sys}: characteristic size of system

f should not vary over dx

dN should be large enough for averaging to be meaningful



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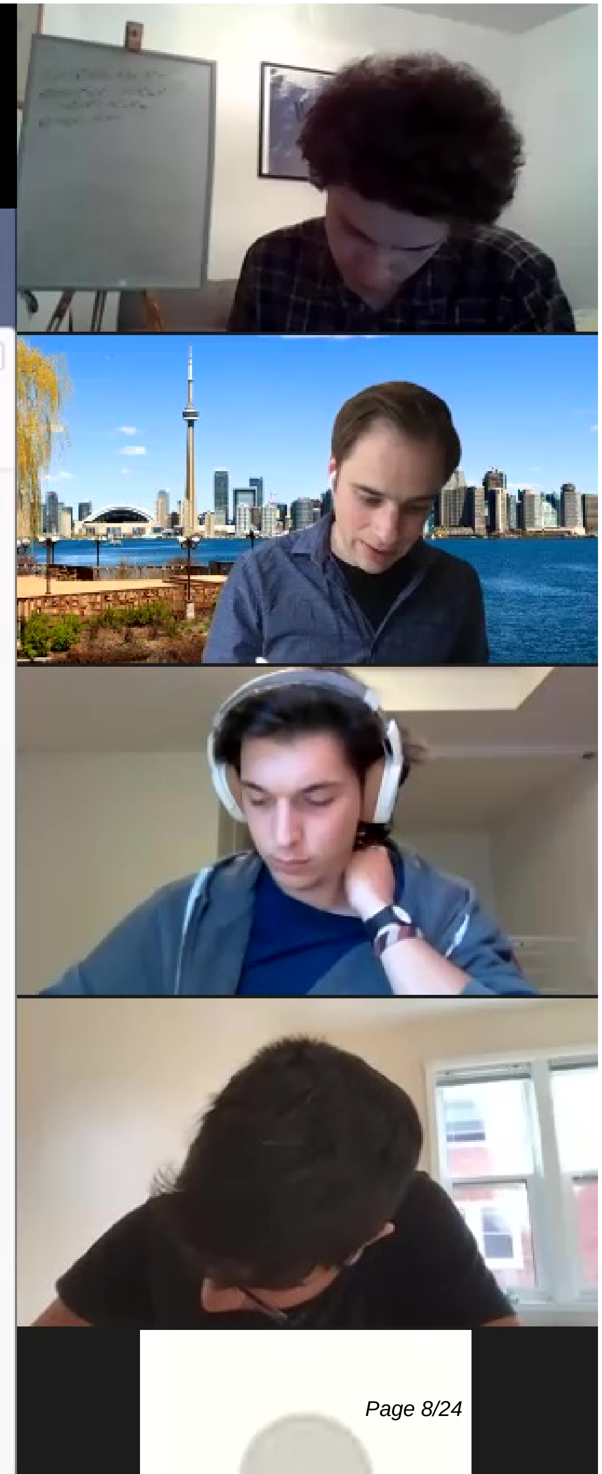
dN should be large enough for averaging to be meaningful

(ii) interparticle forces must be short-range

$$l_{force} \ll dx$$

long range forces: $\vec{F}$

(iii) peculiar motion close to boundary of fluid elements dx leads to "diffusion"



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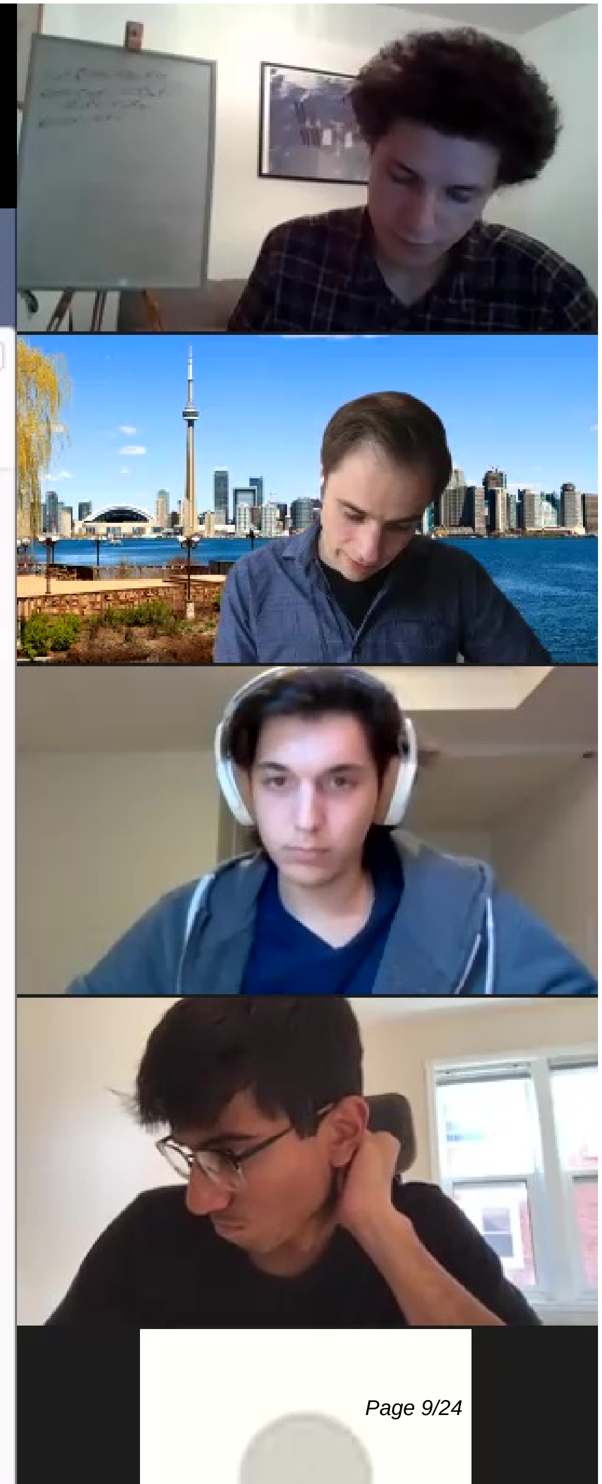
2.3 Viscosity: Navier Stokes Equations

$\rightsquigarrow$ Modify momentum flux density:

$$\pi \to \Pi = \pi - \underbrace{\sigma}_{\text{viscous stress tensor}}, \quad \Pi_{ij} = \rho v_i v_j + p\delta_{ij} \underbrace{- \sigma_{ij}}_{\text{stress tensor}}$$

- friction requires differences in velocity

$\to$ σ should depend on $\frac{\partial v_i}{\partial x_j}$



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- friction requires differences in velocity

  $\longrightarrow$ σ should depend on $\frac{\partial v_i}{\partial x_j}$

  If gradients small $\rightarrow$ only consider 1st order derivatives,

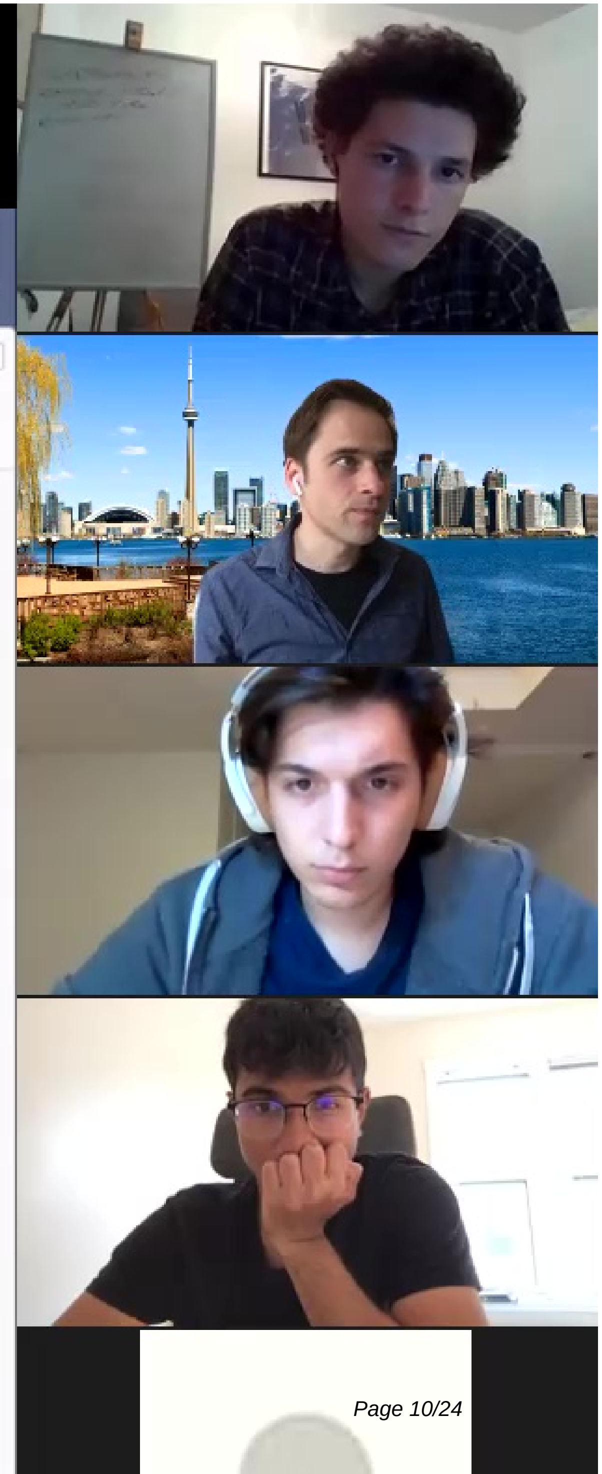
  σ linear in derivatives

- $\sigma = 0$ when the fluid rotates rigidly

  or $v \equiv$ const.

  $\downarrow$ Landau & Lifshitz Fluid Mechanics §15

$$\sigma_{ij} = \eta \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} - \frac{2}{3} \frac{\partial v_k}{\partial x_k} \delta_{ij} \right) + \zeta \frac{\partial v_k}{\partial x_k} \delta_{ij}$$



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shear viscosity coefficient ("dynamic viscosity coefficient")

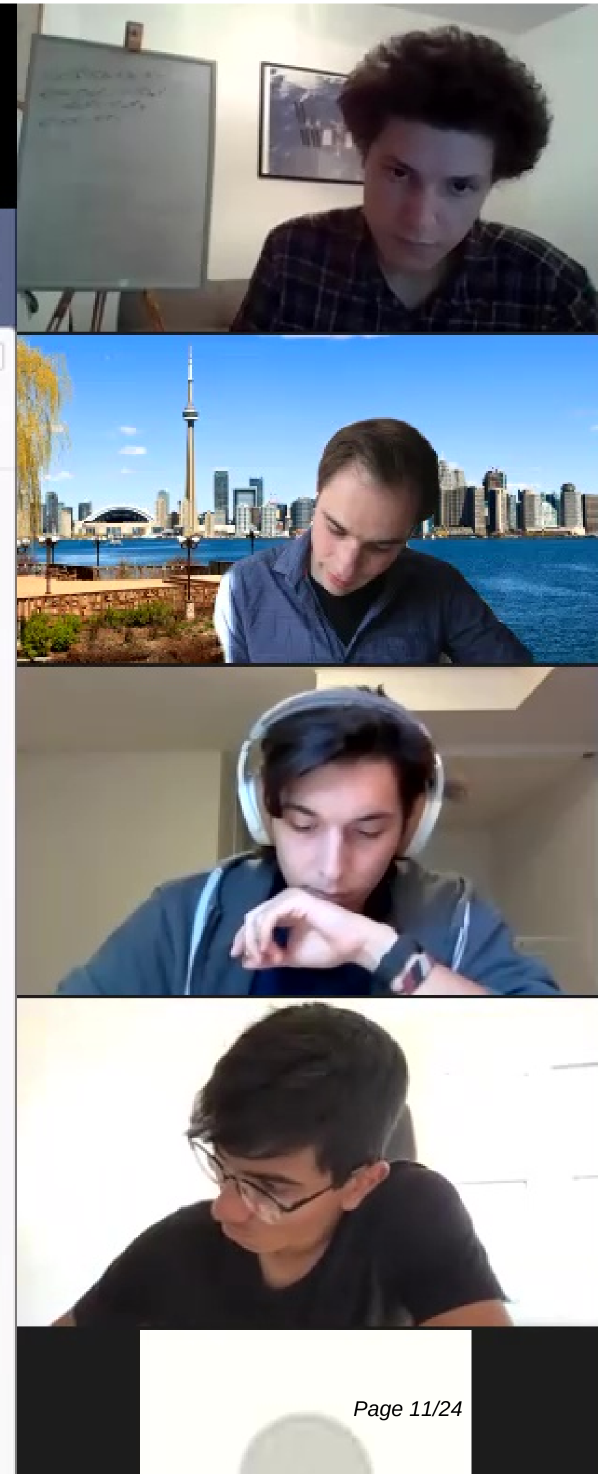
η, ζ independent of velocity ≥ 0

bulk viscosity coefficient

bulk: energy transfer btw translational and internal motions

$\rightarrow$ vanishing for incompressible fluids $\frac{\partial \rho}{\partial t} = 0 \Rightarrow \nabla \cdot \vec{v} = 0$

shear: momentum diffusion through



With the replacement (*) we obtain

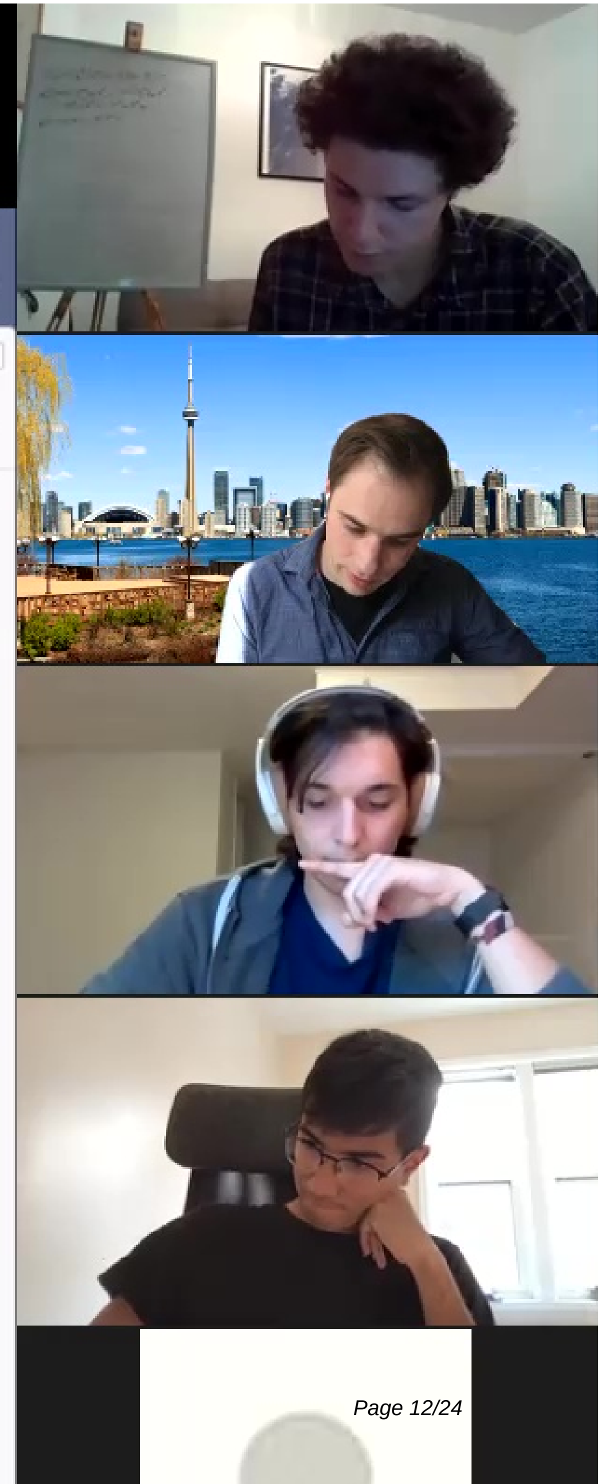
Navier Stokes equations

$$\boxed{\begin{aligned} &\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho v_i) = 0 \\ &\frac{\partial}{\partial t}(\rho v_i) + \frac{\partial}{\partial x_i}\left(\rho v_i v_j - \sigma_{ij}\right) = -\frac{\partial P}{\partial x_i} + \rho F_i \quad (i=1,2,3) \end{aligned}}$$

$$\boxed{\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j}\left[(E+P)v_j - \sigma_{jk} v_k\right] = \rho v_j F_j}$$

Navier (1827)

Stokes (1845)



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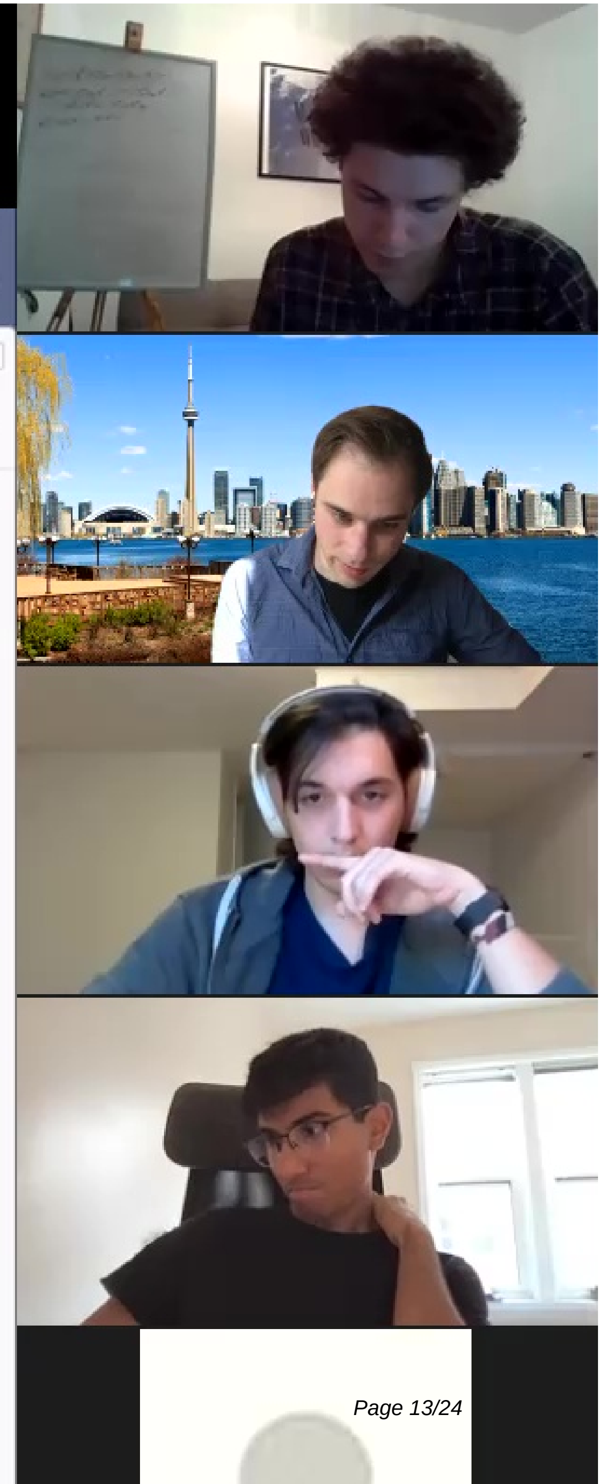
With the replacement (※) we obtain

Navier Stokes equations

$$
\boxed{
\begin{aligned}
&\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho v_i) = 0 \\
&\frac{\partial}{\partial t}(\rho v_i) + \frac{\partial}{\partial x_i}\left(\underline{\rho v_i v_j} - \underline{\sigma_{ij}}\right) = -\frac{\partial P}{\partial x_i} + \rho F_i \quad (i=1,2,3)
\end{aligned}
}
$$

$$
\boxed{\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j}\left[(E+P)v_j - \sigma_{jk} v_k\right] = \rho v_j F_j}
$$

Navier (1827)
Stokes (1845)



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$$\boxed{\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j}\left[(E+P)v_j - \sigma_{jk} v_k\right] = \rho v_j F_j}$$

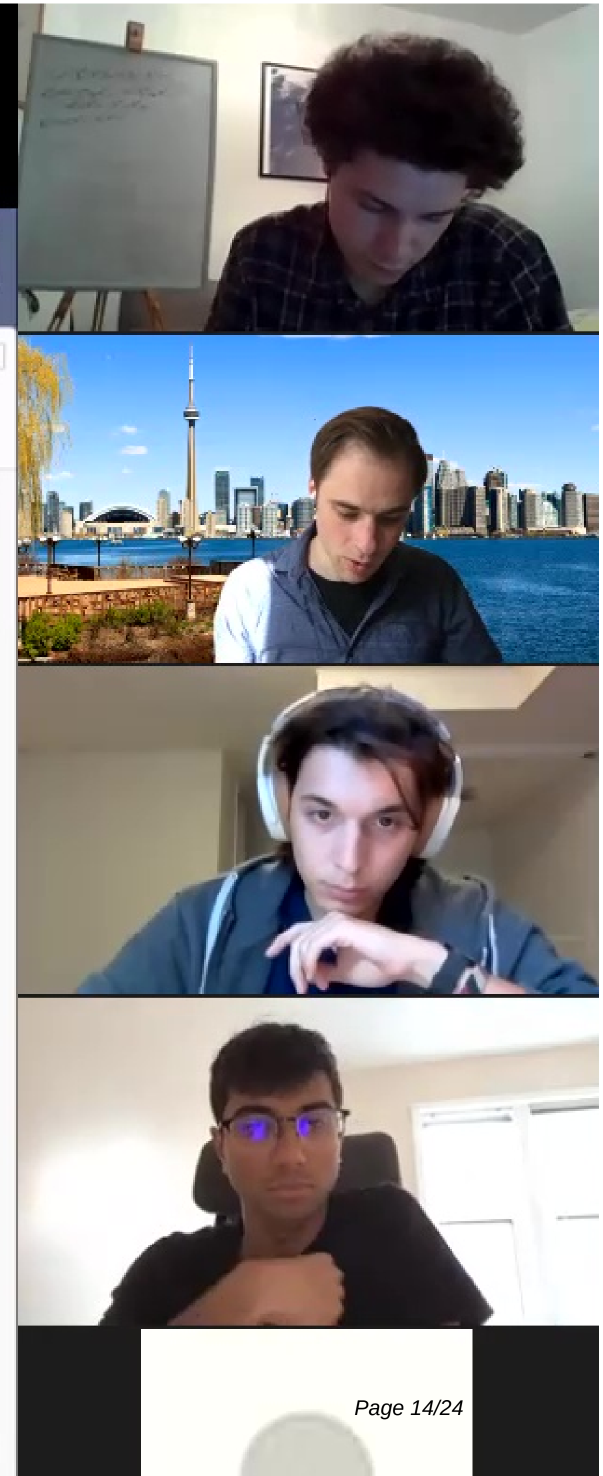
Navier (1827)
Stokes (1845)

Properties of viscous effects

- Viscous timescale:

Assume that viscous effects dominate
(for simplicity, incompressible fluid

$$\Rightarrow \quad \sigma_{ij} = \eta \left(\frac{\partial v_i}{\partial x_j} - \frac{\partial v_j}{\partial x_i} \right)$$



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- Magnitude of effects:

→ <u>molecular viscosity</u> (peculiar motions w.r.t. bulk motion)

$$\nu_{mol} = \lambda \, \tilde{u}_{sys}$$

mean free path

characteristic velocity of peculiar motions

$$t_\nu = \frac{l_{sys}^2}{\lambda \tilde{u}_{sys}}$$

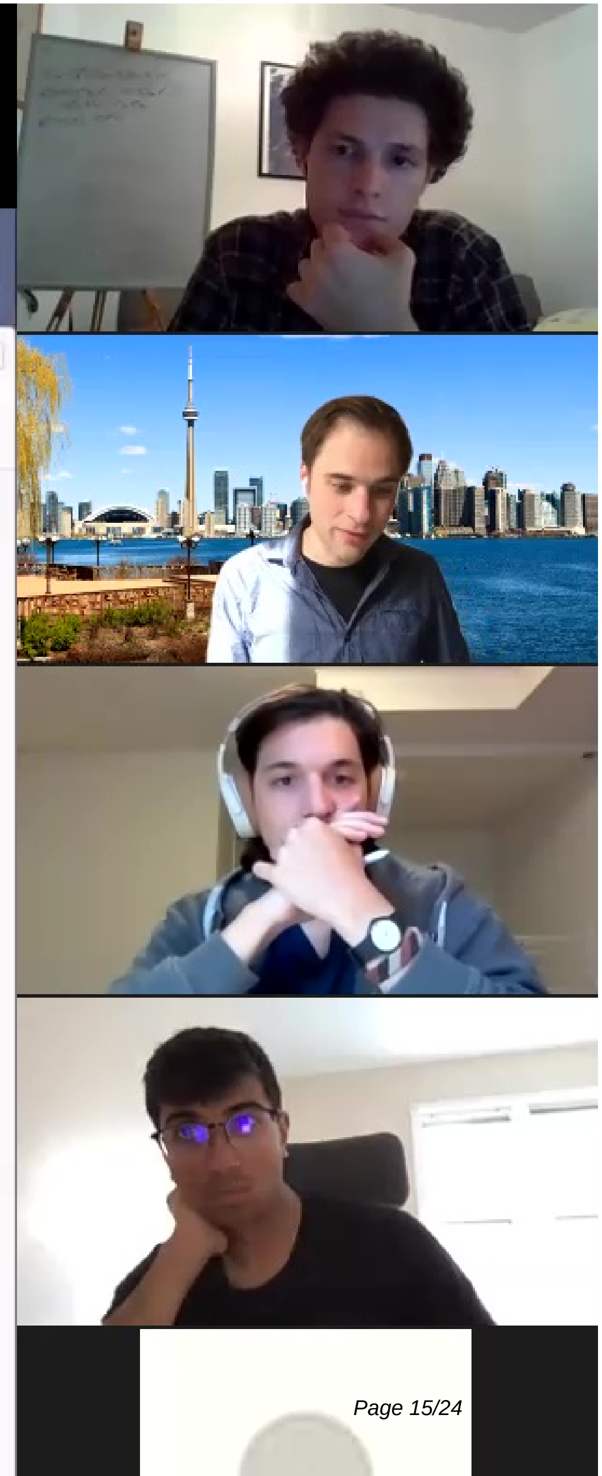
HI cloud $\sim 3 \times 10^{12}$ yr

protostellar disk $\sim 3 \times 10^{14}$ yr

$l_{sys} \sim 10^{19}$ cm

$\lambda \sim 10^{14}$ cm

$\tilde{u}_{sys} \sim 10^{4} \frac{cm}{s}$



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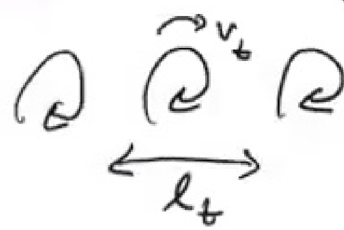
→ <u>turbulent viscosity</u> (turbulent flows within bulk flow)

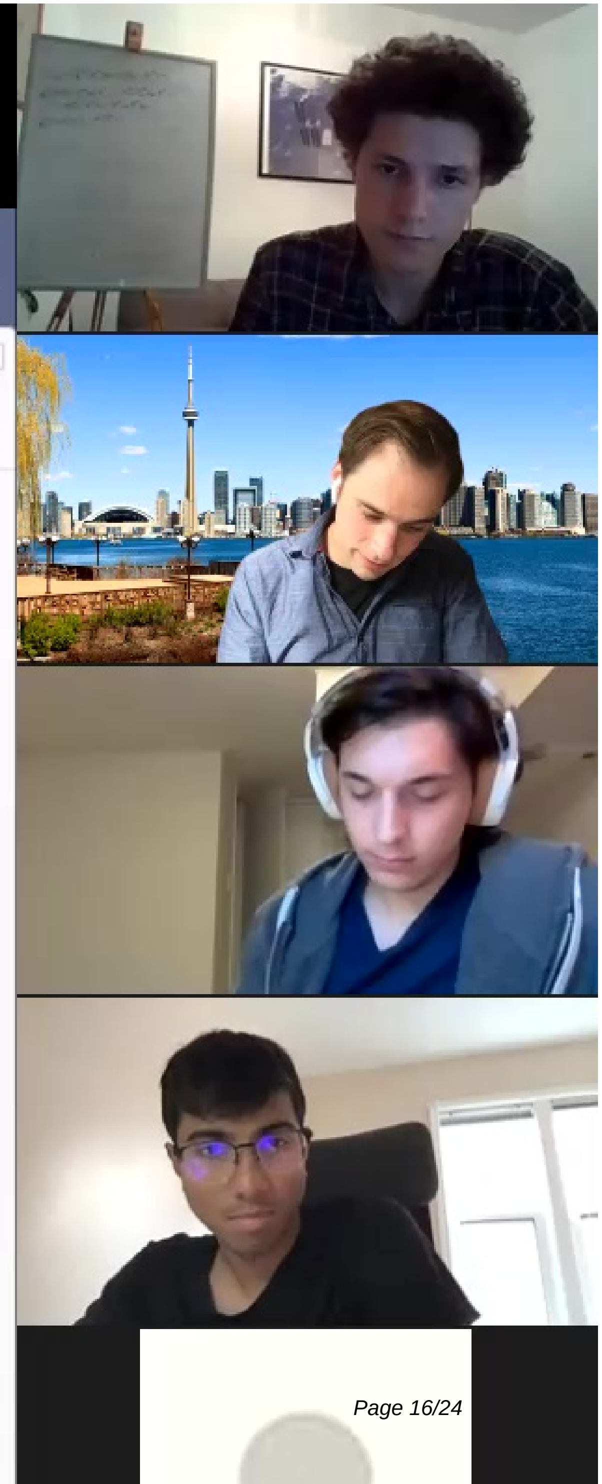
⇝ random motions of eddies with characteristic l_t and velocity v_t

$$\nu = l_t v_t$$



Consider <u>accretion disk</u>:

$l_t \sim h$



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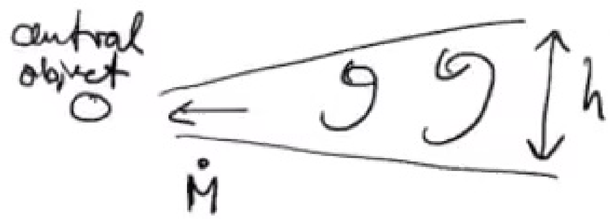
Consider accretion disk:

$\ell_t \sim h$



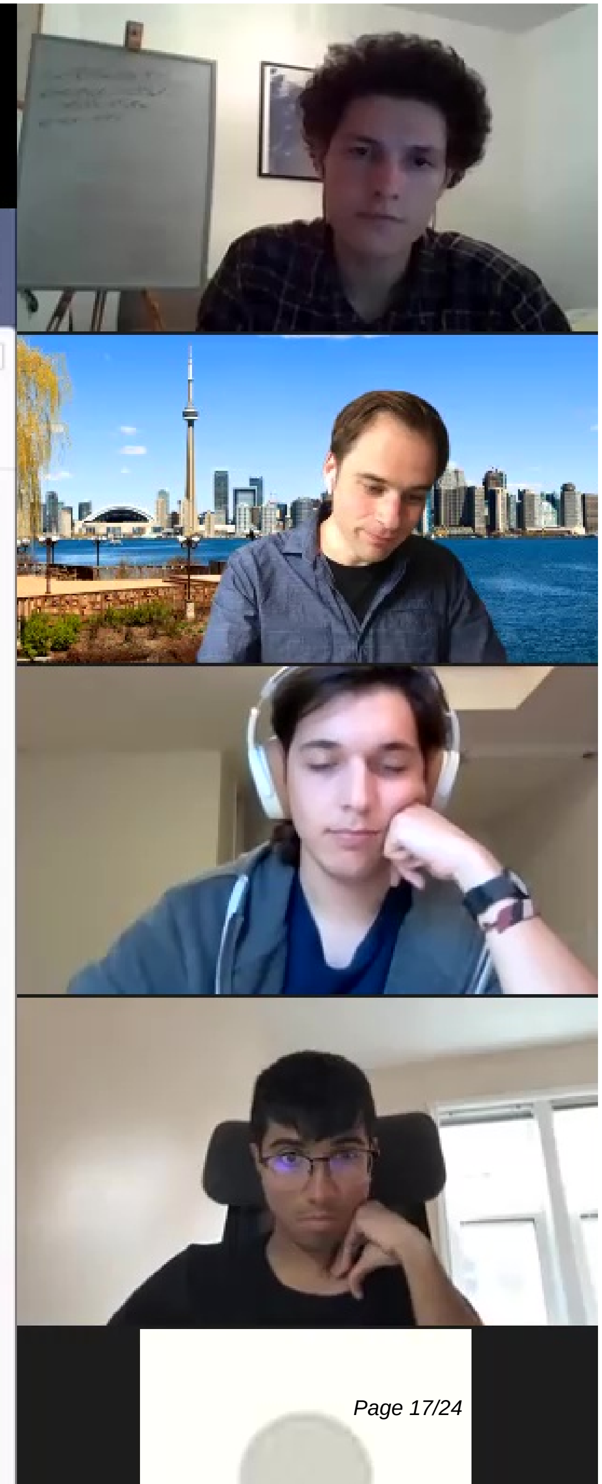
$v_t \sim \alpha \, c_s$

$\in (0,1)$ — sound speed

$\leadsto \nu_t = \alpha \, c_s \, h$

α: "α-viscosity" (Shakura & Sunyaev 1973)

→ source for such disk turbulence



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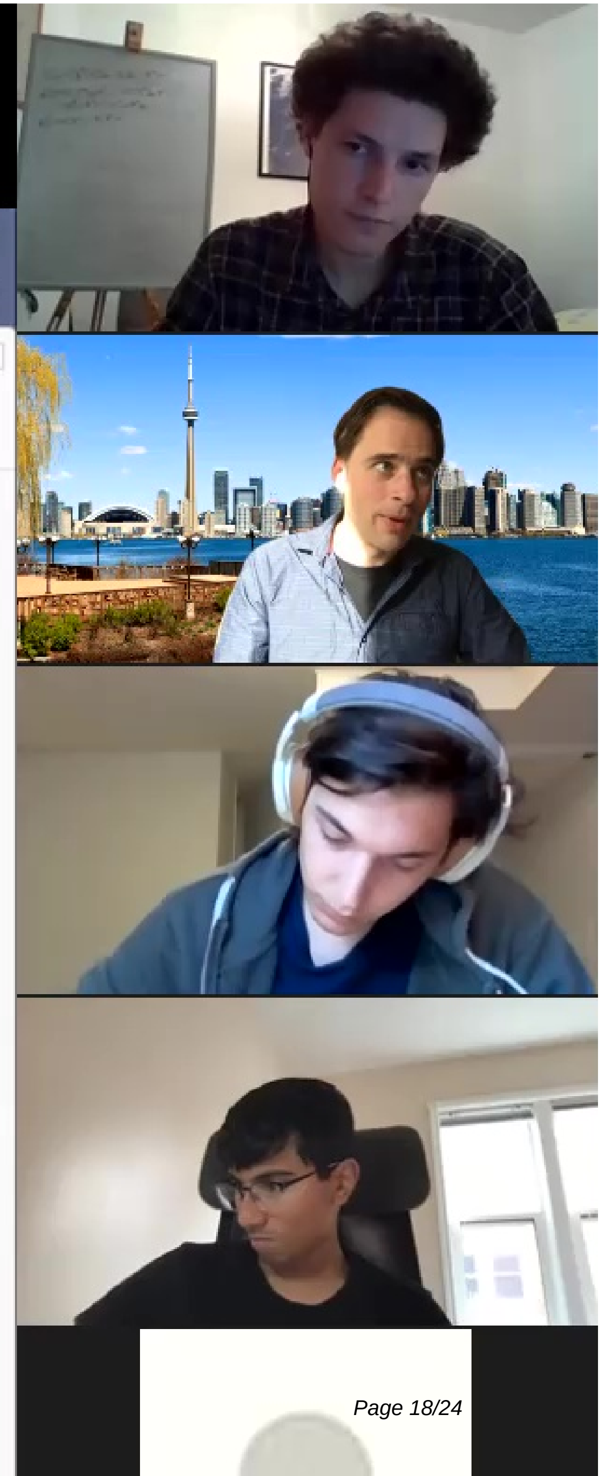
2.4 Magnetohydrodynamics

Ionized medium (plasma) can conduct electric currents $\Rightarrow$ interacts with EM fields

Simplest possible approximation

Magnetohydrodynamics (MHD):

(i) plasma treated as continuous medium,



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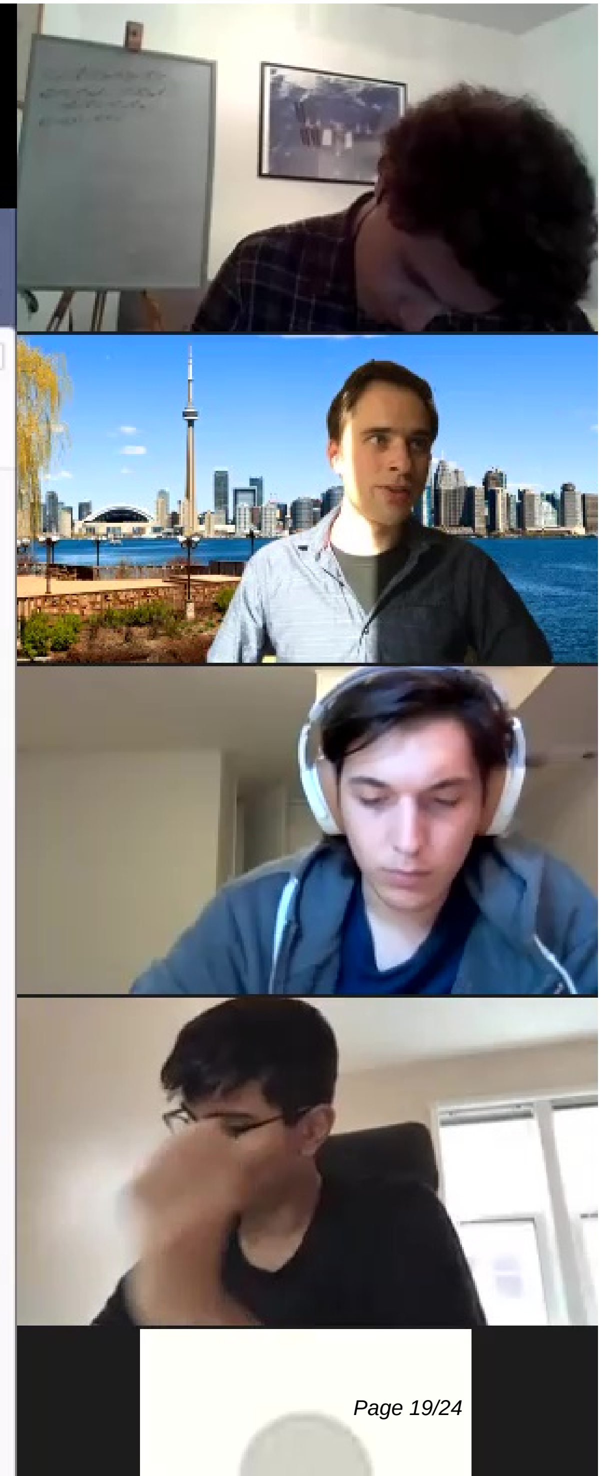
Simplest possible approximation

Magnetohydrodynamics (MHD):

(i) plasma treated as continuous medium, described by Navier-Stokes in absence of EM fields

(ii) positive & negative charges are locally and globally balanced at all times (→ fluid elements are neutral)

(iii) electrons are in statistical equilibrium with ions (same T)



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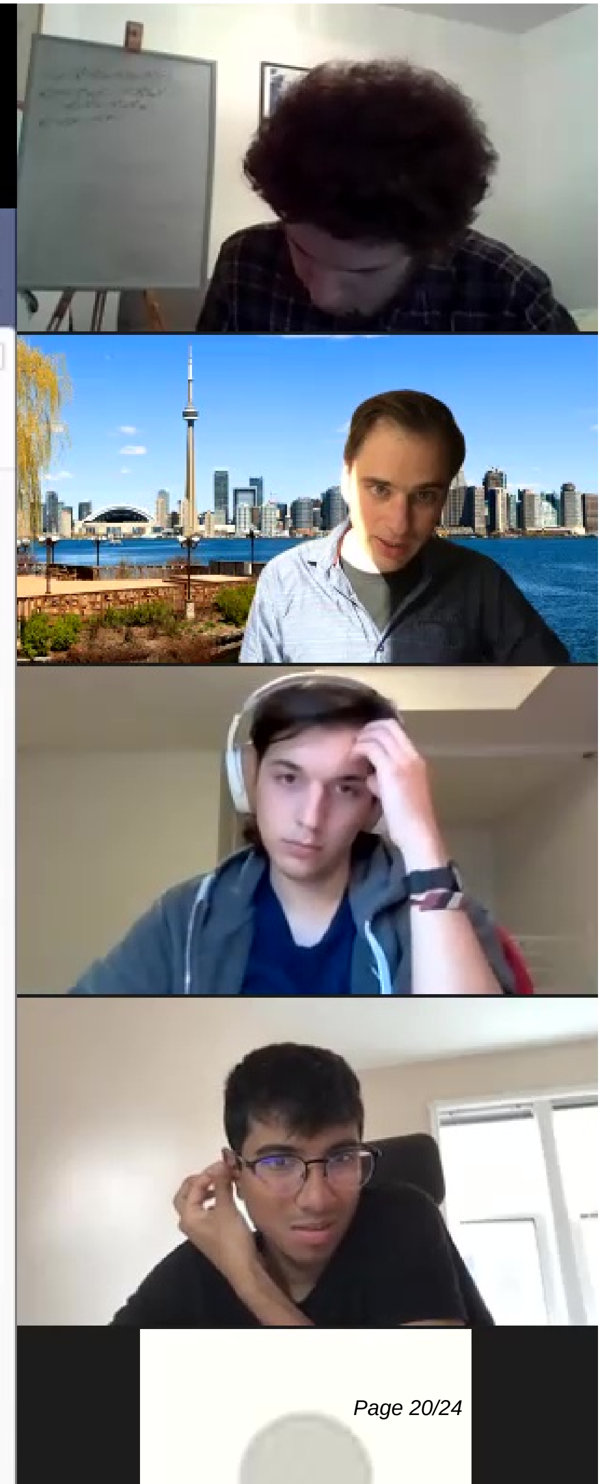
(ii) positive & negative charges are locally and globally balanced at all times
(→ fluid elements are neutral)

(iii) electrons are in statistical equilibrium with ions (same T)

(iv) interparticle collisions frequent enough for all effects of magnetic forces to be instantaneously transferred from e^- to ions & neutral particles (if present)



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Note: for currents to flow, e^- & ions cannot move at the same velocity.

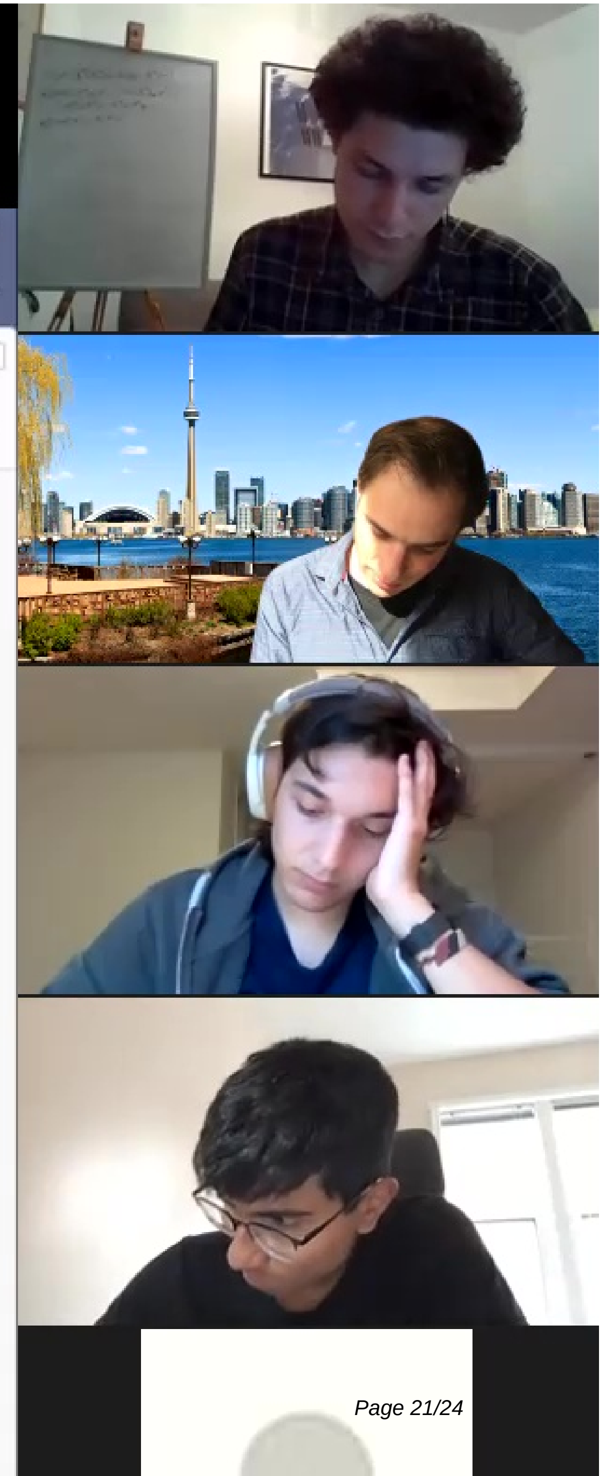
However, the relative drift velocity is so small that it can be neglected (see below)

Vacuum Maxwell eqns:

I $\quad \nabla \cdot \vec{E} = 4\pi q \quad$ (cgs units)

II $\quad \nabla \cdot \vec{B} = 0$

III $\quad \nabla \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t}$



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Plasma approximation:

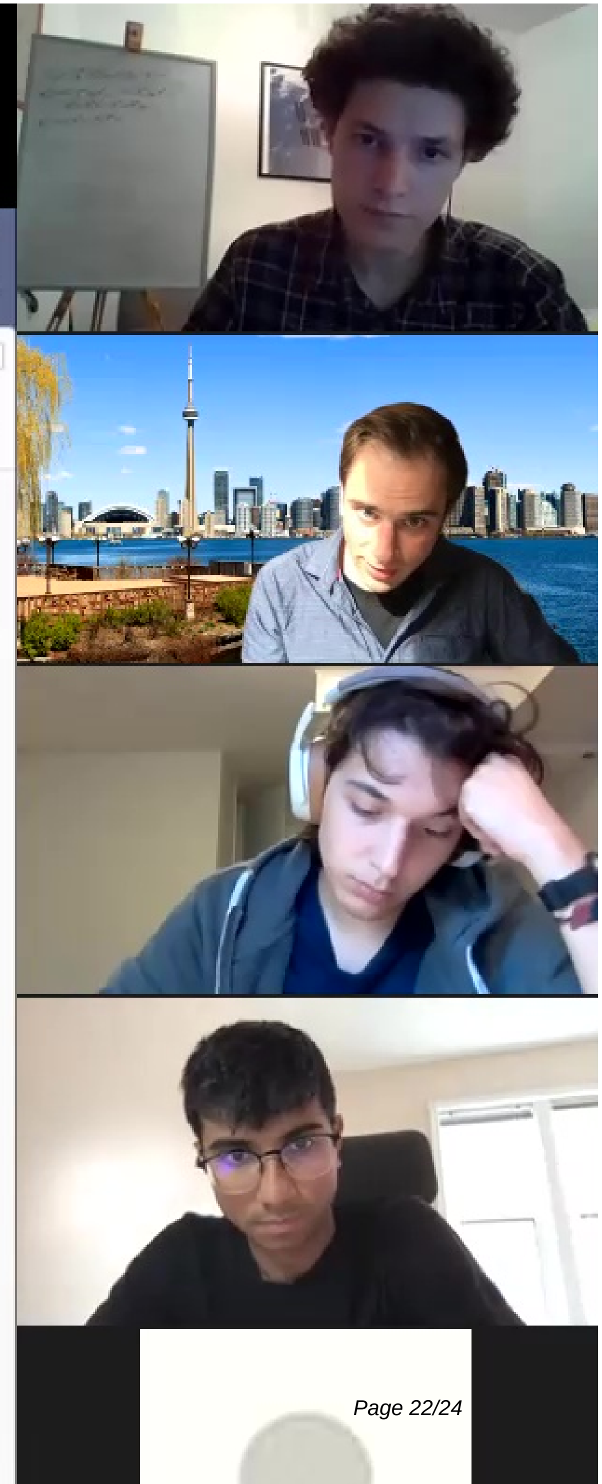
$$\text{III} \Rightarrow \frac{E_{sys}}{\ell_{sys}} \sim \frac{B_{sys}}{c\, t_{sys}} \quad , \quad v_{sys} \equiv \frac{\ell_{sys}}{t_{sys}}$$

$$\frac{1}{c}\frac{\partial \vec{E}}{\partial t} \sim \frac{E_{sys}}{c\, t_{sys}} \sim \frac{B_{sys}\,\ell_{sys}}{c^2 t_{sys}^2} \sim \frac{v_{sys}^2}{c^2}\,|\nabla \times \vec{B}|$$

$$\ll |\nabla \times \vec{B}|$$

assuming non-relativistic plasma

$$|\nabla \times \vec{B}| \approx \frac{B_{sys}}{\ell} \overset{\text{IV}}{\approx} \frac{4\pi}{c}\, q_e n_e\, |v_{drift}|$$



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decelerate, slower element accelerate

With the replacement (*) we obtain

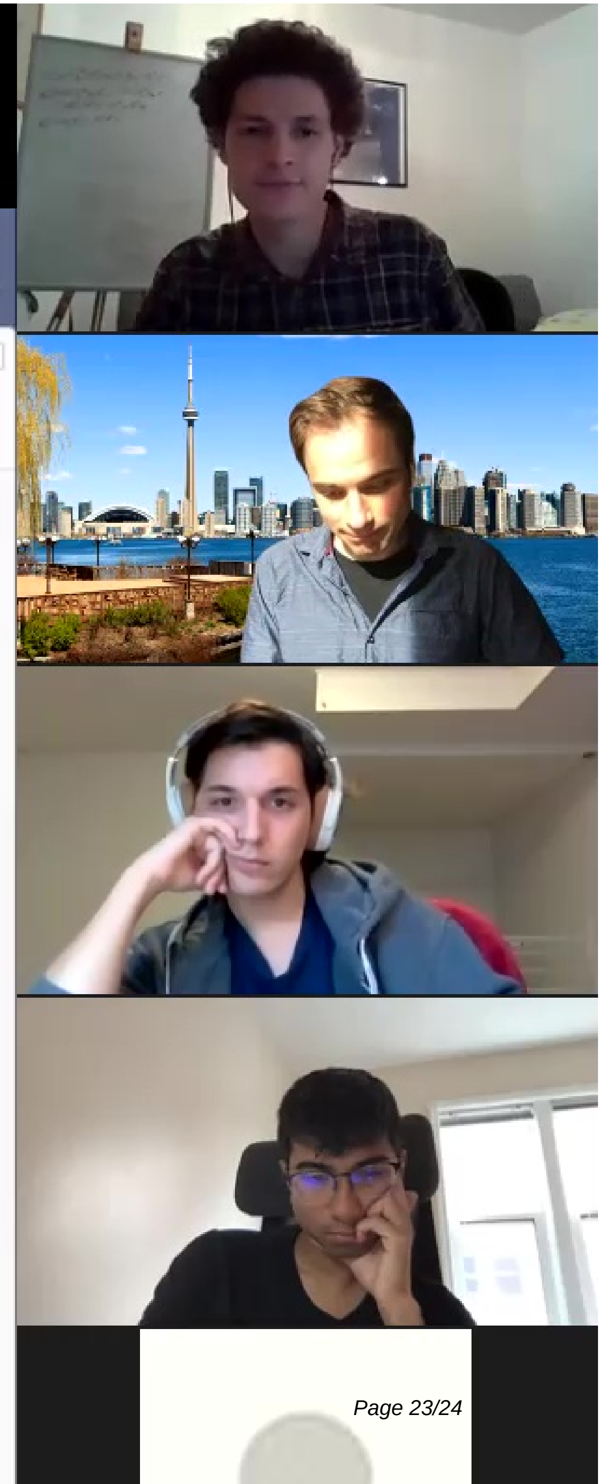
Navier Stokes equations

$$\boxed{\begin{aligned} &\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho v_i) = 0 \\ &\frac{\partial}{\partial t}(\rho v_i) + \frac{\partial}{\partial x_j}(\underline{\rho v_i v_j} - \underline{\sigma_{ij}}) = -\frac{\partial P}{\partial x_i} + \rho F_i \quad (i=1,2,3) \end{aligned}}$$

$$\boxed{\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j}\left[(E+P)v_j - \sigma_{jk} v_k\right] = \rho v_j F_j} \qquad \nabla \Phi$$

Navier (1827)

Stokes (1845) $\qquad \Delta\Phi = 4\pi G \rho(\vec{r})$



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III $$\nabla \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{B}}{\partial t}$$

IV $$\nabla \times \vec{B} = \frac{4\pi}{c}\vec{j} + \cancel{\frac{1}{c}\frac{\partial \vec{E}}{\partial t}} \simeq \frac{4\pi}{c}\vec{j}$$

Plasma approximation:

III $\Rightarrow$ $$\frac{E_{sys}}{l_{sys}} \sim \frac{B_{sys}}{c\, t_{sys}} , \quad v_{sys} = \frac{l_{sys}}{t_{sys}}$$

$$\frac{1}{c}\frac{\partial \vec{E}}{\partial t} \sim \frac{E_{sys}}{c\, t_{sys}} \sim \frac{B_{sys}\, l_{sys}}{c^2 t_{sys}^2} \sim \frac{v_{sys}^2}{c^2}|\nabla \times \vec{B}| \ll |\nabla \times \vec{B}|$$

assuming non-relativistic plasma