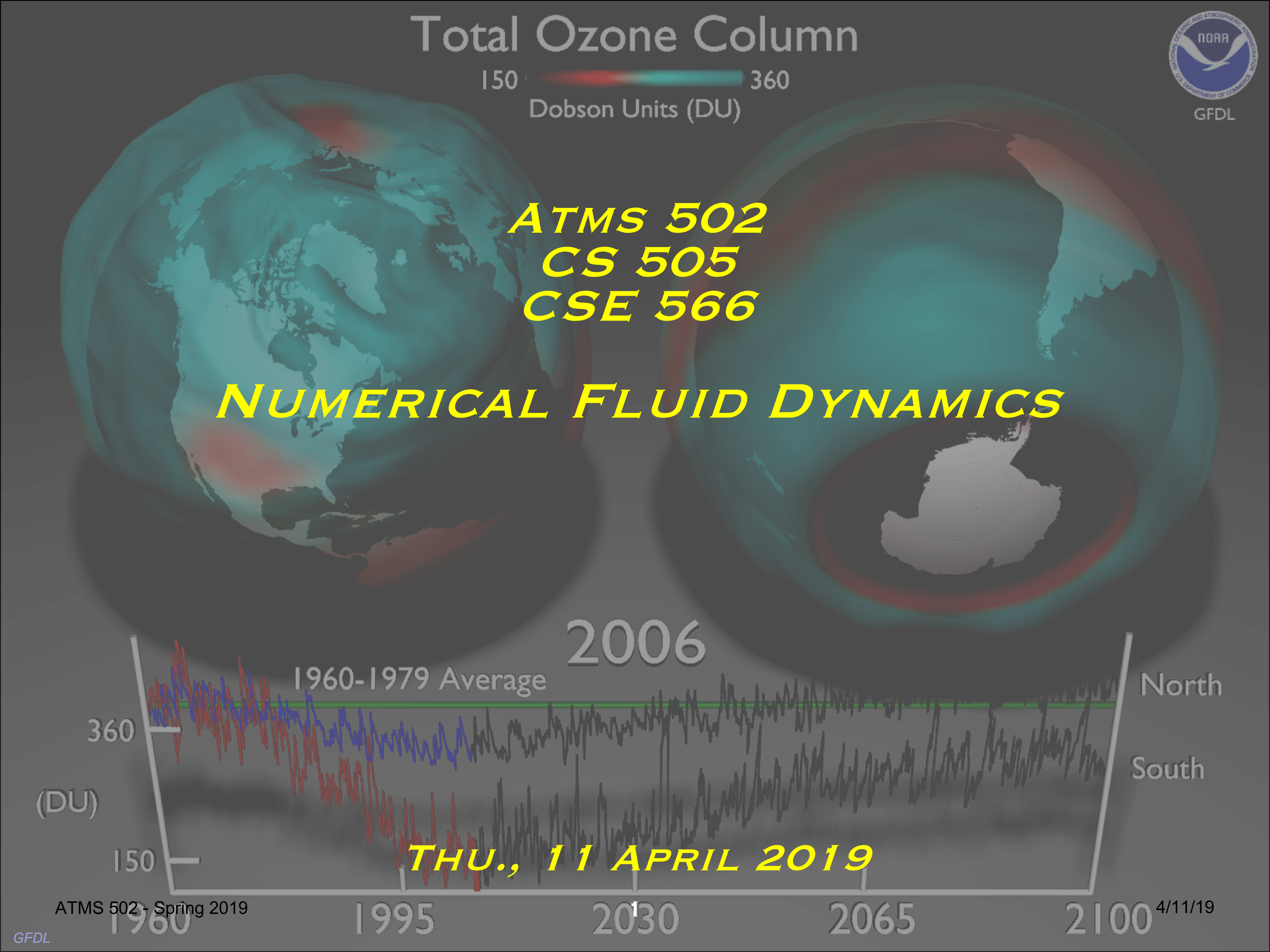
ATMS 502
CS 505
CSE 566

NUMERICAL FLUID DYNAMICS

THU., 11 APRIL 2019



GFDL

ATMS 502
CSE 566

Thursday,
1 April 2019

Class #24

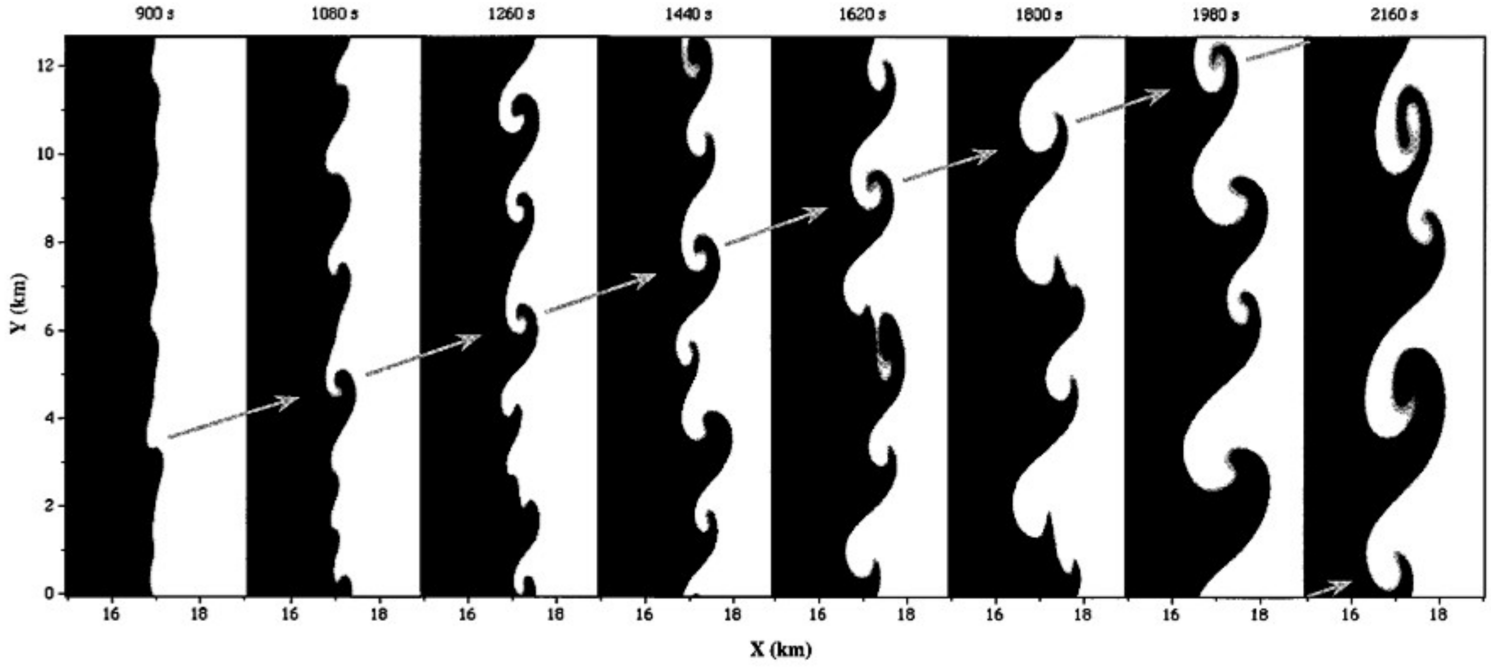
Program #5 is due Tuesday, April 16

Plan for Today

- 1) Using Stampede-2
  - … more effectively
- 2) Program 5, continued
- 3) Lee & Wilhelmson
  - Intro: Density currents, 3D model

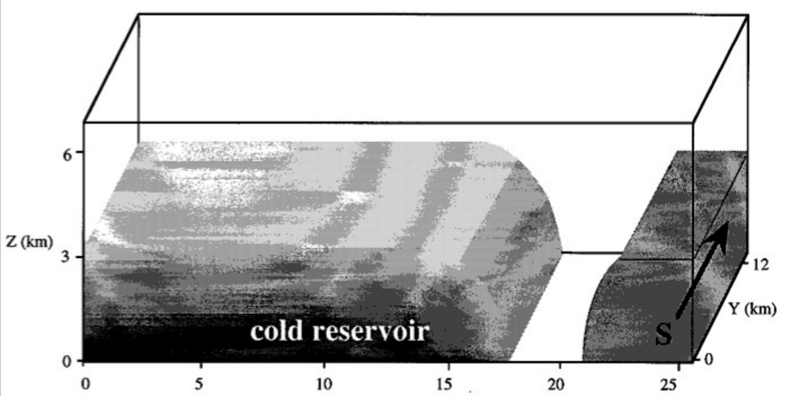
Modeling 3d density currents – background for Program 6

NONLINEAR COMPRESSIBLE FLOW



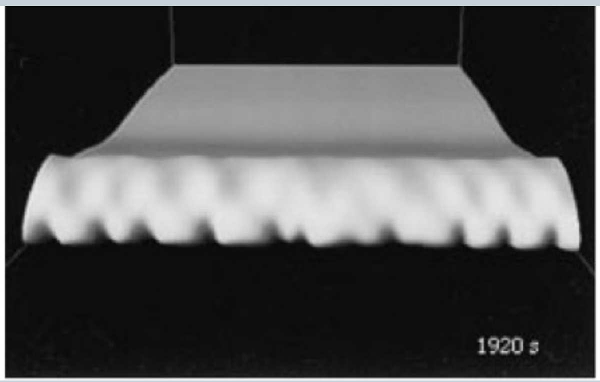
Lee and Wilhelmson (1997)

- Much in common w/computer problem #6 --
- Related to high plains 'landspout' tornadoes
- Configuration:
  - 3-D, Δx=Δy=Δz=100m, dry, quasi-compressible, C-grid
  - Random sfc θ perturbations @ T=0
  - Semi-slip surface: $\left(\frac{\partial u}{\partial t},\frac{\partial v}{\partial t}\right)_{sfc} = \frac{-C_D\left|\vec{V}\right|}{\Delta z}(u,v)$
  - BC: Open X, periodic Y
  - Density current encounters significantly different ***V***



Lee and Wilhelmson (1997)

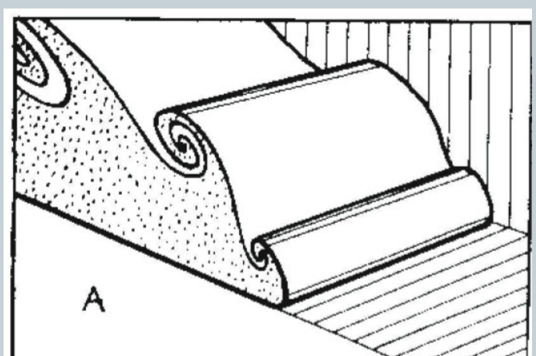
- **Evolution**, step 1:
  - *Random temp. perturbations + semi-slip surface produces **lobe and cleft** instability along leading edge of density current*

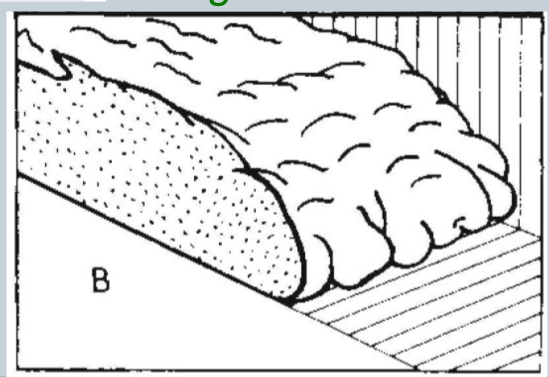


Lee/Wilhelmson Fig. 5: density current leading edge: lobe and cleft instability

Program 6: uses $\Delta U'_{T=0}$

Kelvin-Helmholtz





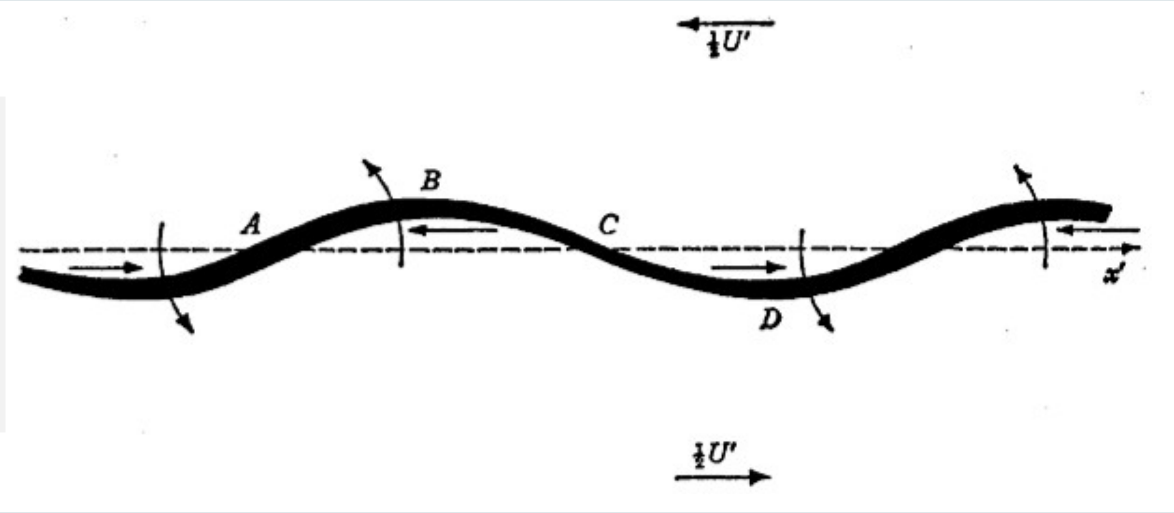
Lobe & Cleft

Simpson (1997)

Lee and Wilhelmson (1997)

- **Evolution**, step 2:
  - *Density current to V>0 region:* ***vortex sheet***
  - *Perturbations on density current lead to* ***horizontal shearing instability*** *(HSI) at leading edge*

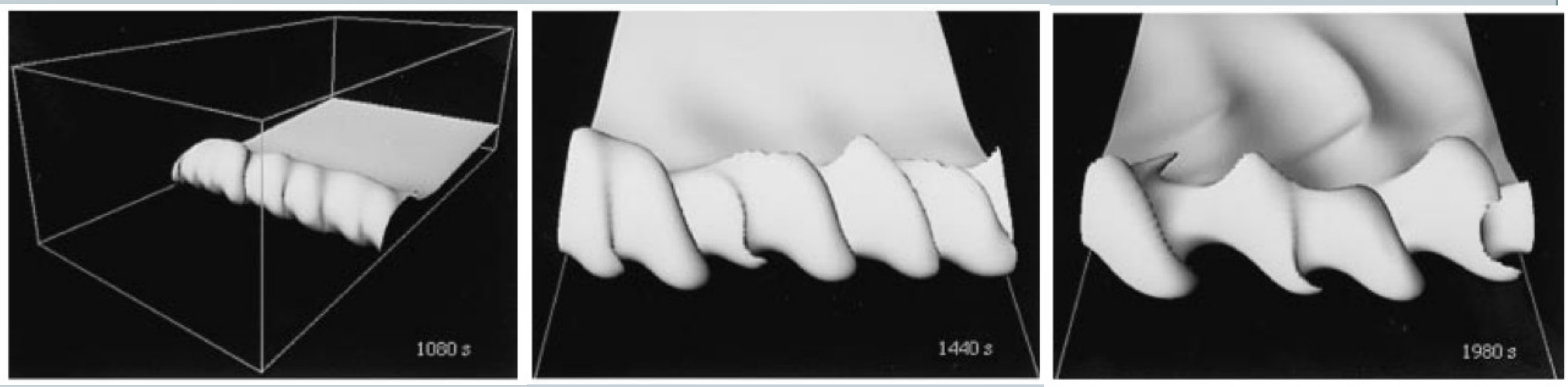
Figure 2: Growth of perturbations on vortex sheet (Batchelor 1967)



Lee and Wilhelmson (1997)

- **Evolution**, step 3:
  - *Circulations with HSI evolve:*
    - *vortex sheet roll up*
    - *subharmonic interaction*
    - *consolidation, dissipation*

Figure 4: Evolution of leading edge of density current.



Transition from wavenumber 8, to 6, to 4

Lee and Wilhelmson (1997)

- **Evolution of leading edge vorticity**

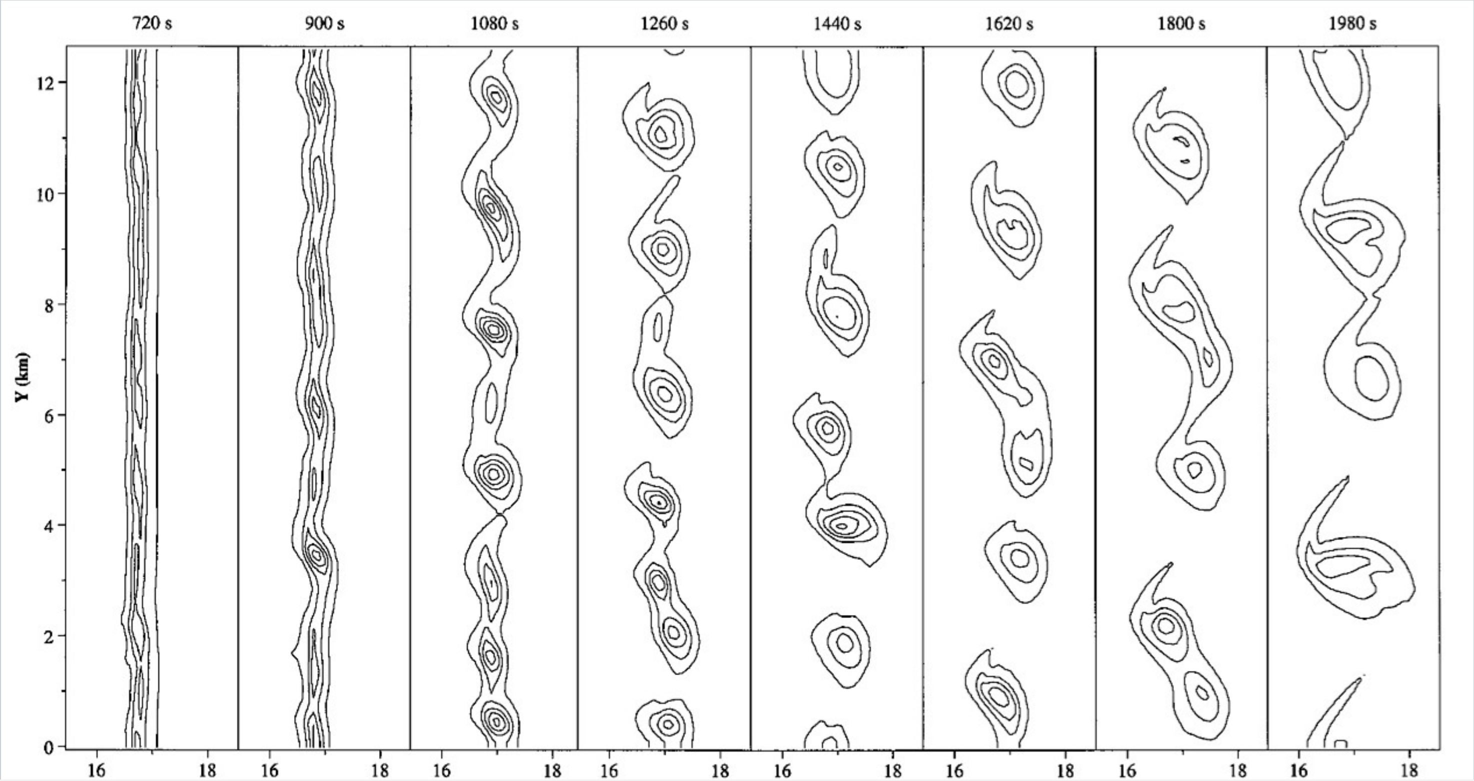


Figure 9: x-y plot of vertical vorticity at leading edge of the density current

Computing: Stampede

MORE ON:
OUR CLASS COMPUTING RESOURCE

DETAILS:
HTTPS://WWW.TACC.UTEXAS.EDU/SYSTEMS/STAMPEDE2

Backups!

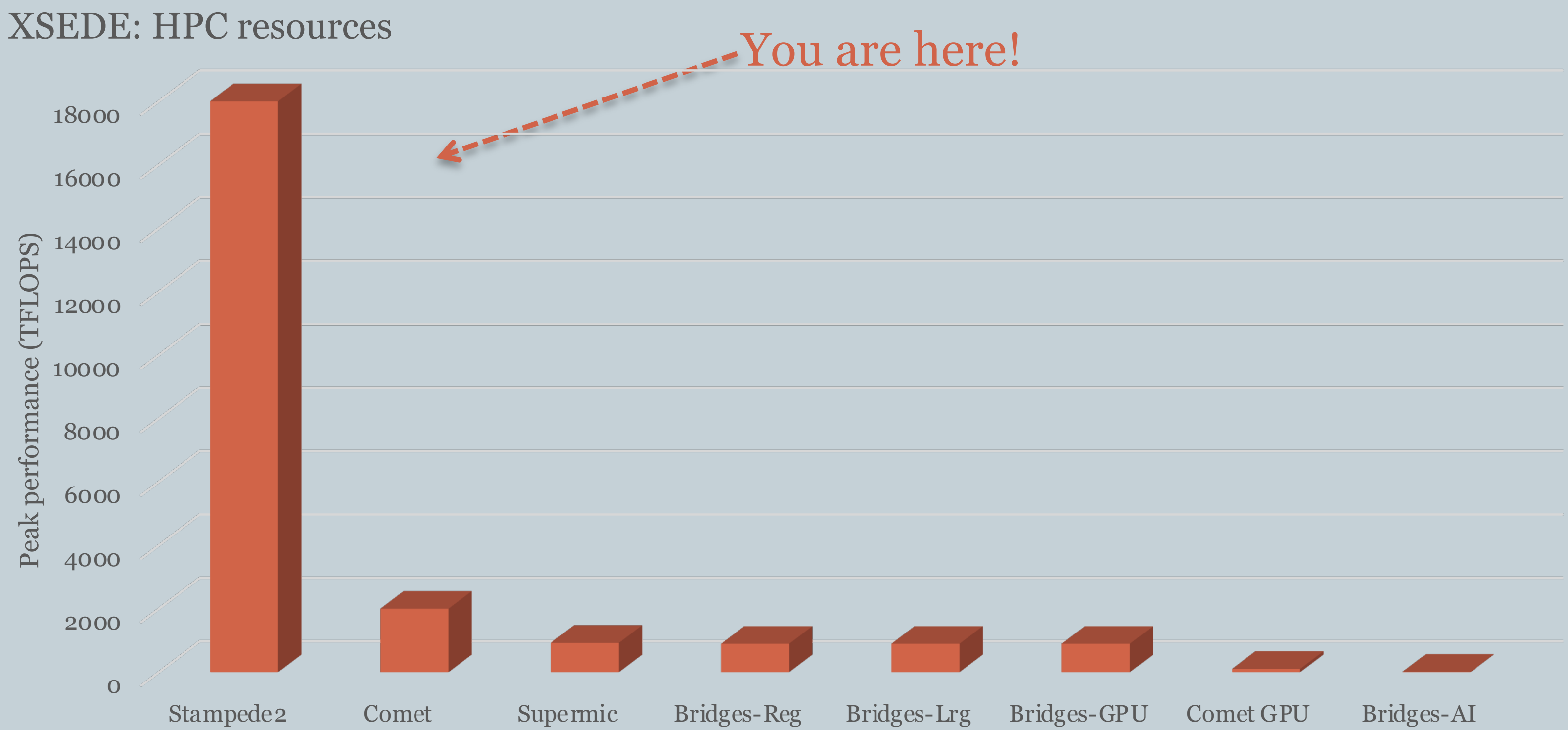

```
Stampede is currently in emergency maintenance mode.
Remote access will be unavailable until after the
maintenance is complete.

Connection closed by 129.114.62.13
```

- Please do backups!
  - You can use the Work or Scratch space for backups
  - Also available: the Ranch mass store system
  - Remember ***only*** the Home directory is **backed up** by TACC
  - Quick backup: *cp* yourfile *$WORK*

Xsede HPC resources

- Resources: https://portal.xsede.org/allocations/resource-info
- Resource monitor: https://portal.xsede.org/resource-monitor



Stampede-2: By the numbers

- Stampede-2: About 18 PFLOPS *(#12)*
  - FLOPS = Floating Point Operations per Second
  - 10^6 = mega, 10^9 = giga, 10^{12} = tera, 10^{15} = peta, 10^{18} = exa
  - Peta = quadrillion (fast).
- For comparison … *www.top500.org*
  - Blue Waters @Illinois ~ 13 PFLOPS
  - Cheyenne (NCAR - Atmospheric research) ~ 5 PFLOPS (#26)
  - Wuxi Nat'l Supercomputing Center ~ 125 PFLOPS (#3)
  - DOE/Oak Ridge Nat'l Lab: Summit ~ 201 PFLOPS (#1)
- Summary
  - 4200 KNL *nodes* • 1736 Skylake *nodes* • 369,000 *cores*
  - *Only* 31 PBytes of storage!

Stampede-2: Storage summary

- You may still do everything in your *home* directory
  - Typing "cd" does a *change directory* to home.
  - Quota: 10 GB, 200k files. $HOME *is backed up for you.*
- There are other directories: *(all are Lustre filesystems)*
  - $WORK
    - "*cdw*" same as *cd $WORK*
    - Quota: 1024 GB, 3M files. It is *not* backed up.
    - To copy a file to Work: *cp filename $WORK*
  - $SCRATCH
    - "*cds*" same as *cd $SCRATCH*
    - Quota: None (sort-of)! *Not* backed up, and is occasionally *purged.*
    - To copy a file to Scratch: *cp filename $SCRATCH*

Stampede-2 : Login vs. compute nodes

- *Login nodes*:
  - Shared with others! Could be slow.
  - Details: On each node …
    - 2 sockets, 14 cores each, 28 cores total
    - Each core runs at 2.7 GHz
  - Use it …
    - Compiling, running *small* jobs, examining run output.
  - Large multi-processor jobs are run in *batch*.

- *Using compute nodes interactively* (link)
  - *idev* (interact. development): http://portal.tacc.utexas.edu/software/idev
  - *idev* -p normal -m 150 (normal queue, 150 min)

Stampede-2 – use summary

- Working in your home directory is fine.
  - But make occasional copies of your files to $WORK
  - Remember HOME is backed up; WORK is not.
- Future
  - Anticipate the day (by program 6, if not program 5) when you will need to do you work in $WORK
    - you go there by *cd $WORK* or by typing *cdw*
    - when that day comes, working in $WORK, you will need to regularly copy critical (source code, script) files back HOME.
- Consider …
  - Mailing yourself or otherwise occasionally copy your code back to your PC…. it is good to have a copy if Stampede goes down.

Stampede-2 – speeding up your work

- Consider *idt* instead of converting to GIFs *(use X11)*
- Only *make clean* if you change OPTIONS in *Makefile*
- Script *the steps you are doing repeatedly:*

```
#!/bin/tcsh
rm  pgm5  gmeta  # to not run old pgm5 -or- plot old files
make pgm5
./pgm5 << TheEnd
10
L
TheEnd
idt gmeta   or   ~tg457444/502/Tools/metagif  gmeta  -all  -zip
```

Put your text in "run"...
chmod u+x run
To use: ./run

Program #5

2D NONLINEAR, COMPRESSIBLE FLOW *CONTINUED*

Program 5 array sizes

- Array sizes
  - Need 1 ghost point per *U, W, P* array; 2 for theta (e.g. "s1")
  - So in Fortran, I dimensioned 0:nx+1, 0:nz+1 for *everything*
    - wait, what? What about staggering?
      - we don't need X ghost points for U *(symmetry boundary)*
      - we don't need Z ghost points for W (rigid lids top & bottom)
    - pressure & theta
      - this provides 1 ghost point (X and Z) for P
      - theta: I used *one* ghost point per 2D theta variable, and set the extra point in the 1d array before passing to *advect1d*

Program 5 coding - general

- Theta (2 time levels)
  - Is still forward in time. Everything to do with theta uses *dt*
  - Advection/diffusion is (1:nx, 1:nz) but needs 2 ghost points
- *U, W, P*
  - centered time differencing; each array has 3 time levels
  - pressure is strange: nothing uses *p2* other than update step
  - integration loops:
    - U: 2:nx, 1:nz (i=1 and i=nx+1 set w/symmetry conditions)
    - W: 1:nx, 2:nz (w=0 always at k=1, k=nz+1)
    - P: 1:nx, 1:nz

Program 5 - specifics

- Advection
  - Theta advection is unchanged! except: piecewise linear
  - Add advection of U and W somewhere in your 2D advection.
- PGF
  - It only needs *tstep* – not **dt**! (PGF involves only u, w, p)
  - U uses (n-1) dp/dx term; finishes updating u3 to time (n+1)
  - W uses (n-1) dp/dz term + buoyancy, takes w3 to (n+1)
  - dp/dx uses density, (n+1) du/dx and dw/dz: u3, w3 => p3
- Diffusion
  - Watch array index bounds – they vary by variable! (last slide)
  - U, W use *tstep* • Theta uses *dt* • *2nd-order* expression!!

Overview: Wave equations in Geophysical Fluid Dynamics

***REFERENCES*:**

- **DURRAN CHAPS. 1,7**
- **HALTINER & WILLIAMS CHAP. 1,2**
- **FERZIGER AND PERIC *(2002, 3RD EDITION)***

Reference information

- A020 – Inviscid flow
- A021 – Euler equations
- A022 – Momentum equation in CFD
- A023 – Pressure equation and Exner form in CFD
- A024 – Continuity equation in CFD
- A029 – Compressibility
- A031 – Boussinesq approximation

Eulerian vs. Lagrangian

- The Eulerian viewpoint:
  - select a given location x,y,z
  - observe how the properties (e.g., velocity, pressure and temperature) change there.
- The Lagrangian viewpoint: a fluid particle is followed
  - As the fluid particle travels, observe the change of properties at its location –
    - position + T, ρ, p(x, y, z, t)
    - where x, y, and z represent a particular particle/object.

OU ecourse on fluid mechanics

- *Leonhard Euler was a Swiss mathematician and physicist*

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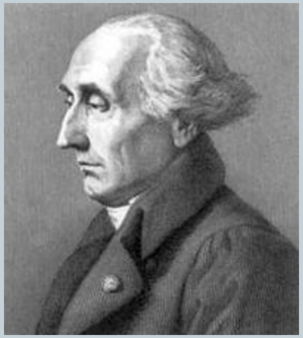
- *Joseph-Louis Lagrange was a mathematician and astronomer*



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Total derivatives following the flow *include* advective terms:

$$\frac{d\phi}{dt} \equiv \frac{\partial \phi}{\partial t} + \vec{V} \bullet \vec{\nabla}\phi$$

Momentum equation

- Forms of the inviscid momentum equations:

Full set, ***p***	$\frac{d\vec{V}}{dt} = -\frac{1}{\rho}\vec{\nabla}p - f\hat{k}\times\vec{V} - g\hat{k}$
Full set, π	$\frac{d\vec{V}}{dt} = -c_p\theta\vec{\nabla}\pi - f\hat{k}\times\vec{V} - g\hat{k}$
Boussinesq, π	$\frac{d\vec{V}}{dt} = -c_p\theta_0\vec{\nabla}\pi - f\hat{k}\times\vec{V} - g\hat{k}$
Shallow water	$\frac{d\vec{V}_h}{dt} = -g\vec{\nabla}_h h - f\hat{k}\times\vec{V}$

Pressure equation

- Forms of the pressure equation:

Compressible *Klemp and Wilhelmson*	$\frac{\partial \pi'}{\partial t} + \frac{\bar{c}^2}{\bar{\rho} C_p \bar{\theta}_v^2}\left[\frac{\partial}{\partial x}\left(\bar{\rho}\bar{\theta}_v u\right) + \frac{\partial}{\partial y}\left(\bar{\rho}\bar{\theta}_v v\right) + \frac{\partial}{\partial z}\left(\overline{\rho \theta_v} w\right)\right] = f_\pi$
Compressible *Durran (Euler equations)*	$\frac{d\pi}{dt} = -\frac{R\pi}{c_v} \nabla \cdot \vec{v}$
Quasi-compressible	$\frac{\partial p}{\partial t} = -c_s^2\left[\bar{\rho}\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) + \frac{\partial\left(\bar{\rho} z\right)}{\partial z}\right]$
Boussinesq *diagnostic*	$\nabla^2 p' = \rho_0 \vec{\nabla} \cdot \vec{F} = \rho_0 \vec{\nabla} \cdot \left\{-\vec{v} \cdot \vec{\nabla} v - g\frac{\rho'}{\rho_0}\vec{k}\right\}$

Continuity equation

- Forms of the continuity equation:

Compressible	$\frac{\partial \rho}{\partial t} = -\vec{\nabla} \bullet \rho \vec{V}$	*Full form*
Anelastic	$\nabla \cdot \overline{\rho} \vec{V} = 0$	*Base state $\rho(z)$*
Boussinesq	$\vec{\nabla} \bullet \vec{V} = 0$	*ρ variations retained only in buoyancy terms*
Incompressible	$\vec{\nabla} \bullet \vec{V} = 0$	*ρ =constant*

Some approximations

- Incompressibility
  - *Eliminates dρ/dt, u•dρ/dx*

- Inviscid (Euler) flow
  - *Eliminates friction terms*
- Hydrostatic balance
  - *Eliminates dw/dt, u•dw/dx terms*

- Boussinesq
  - Density variations *neglected* in mass balance, but *retained* where connected to gravity.
    - ✓ Inappropriate if large changes in mean density over fluid depth

$$\frac{d\vec{V}}{dt} = -\vec{\nabla}\left(\frac{\mathrm{p}}{\rho_0}\right) - g\left(\frac{\rho - \bar{\rho}}{\rho_0} \text{ or } \frac{\theta - \bar{\theta}}{\theta_0}\right)\vec{k} \quad \text{and} \quad \vec{\nabla} \cdot \vec{V} = 0$$

Approximations (1)

- Incompressibility
  - Constant density - appropriate for liquids, and gases for Mach number below 0.3 *(FP).*
- *Ferziger and Peric (p. 184):*

"The major difference between the equations of compressible flow and those of incompressible flow is their mathematical character. The compressible flow equations are hyperbolic which means that they have real characteristics on which signals travel at finite propagation speeds; this reflects the ability of compressible fluids to support sound waves.

"By contrast .. the incompressible equations have a mixed parabolic-elliptic character …

"The difference can be traced to the lack of a time derivative term in the incompressible continuity equation. The compressible version contains the time derivative of density."

Notes

Approximations (2)

- Inviscid (Euler) flow
  - Navier-Stokes equations with no viscosity
  - Far from solid surfaces ... or ...
    Fluid cannot stick to walls
  - Slip possible at solid boundaries
  - Used to study high Mach # compressible flows
- Hydrostatic balance
  - dw/dt = 0; *dp/dz balances buoyancy*
- Anelastic
  - Density in continuity eqn is f(*z*) only: $\vec{\nabla} \cdot \left(\overline{\rho} \vec{v} \right) = 0$

Boussinesq approximation

- Boussinesq equation forms

$$\left.\begin{array}{l} \dfrac{d\vec{v}}{dt} = -\vec{\nabla}P + b\vec{k} \\ \dfrac{db}{dt} = -N^2 w \\ \vec{\nabla}\cdot\vec{v} = 0 \end{array}\right\} \textit{where} \left\{\begin{array}{l} P = \dfrac{p}{\rho_0} \\ b = -g\dfrac{\rho - \overline{\rho}}{\rho_0} \\ N^2 = -\dfrac{g}{\rho_0}\dfrac{d\overline{\rho}}{dz} \end{array}\right. \textit{or} \left\{\begin{array}{l} P = c_p\theta_0\pi' \\ b = -g\dfrac{\theta - \overline{\theta}}{\theta_0} \\ N^2 = \dfrac{g}{\theta_0}\dfrac{d\overline{\theta}}{dz} \end{array}\right.$$

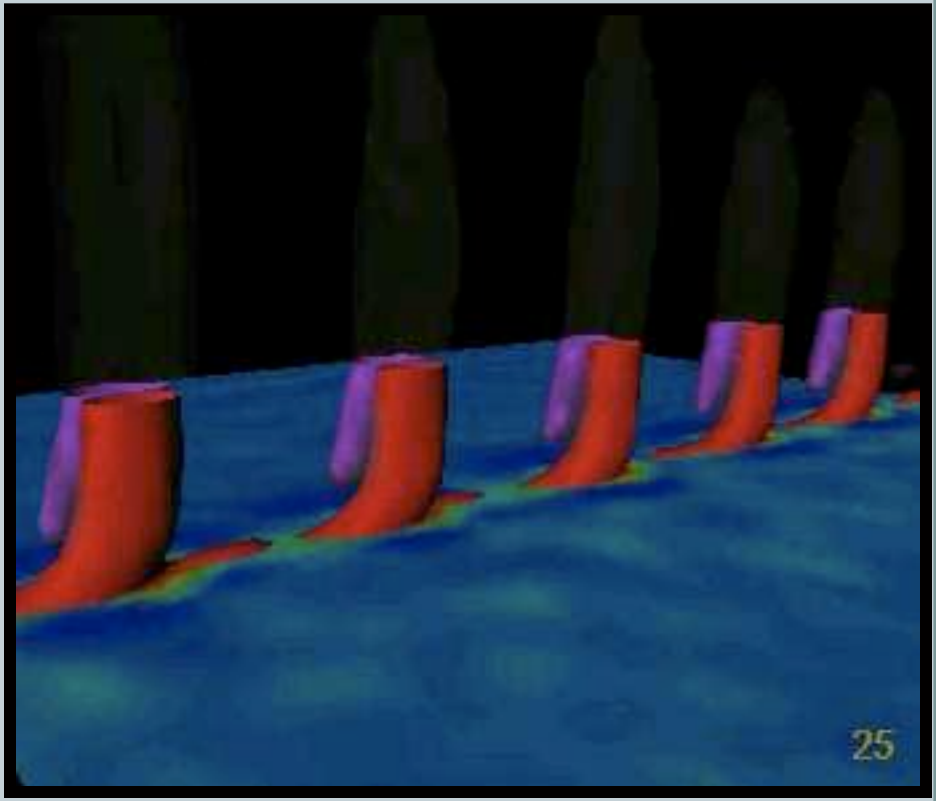
  - Linearizes pressure gradient terms
    - Inappropriate if large changes in mean density over fluid depth
  - Durran: often *"easier to satisfy this constraint"* – $\theta \sim \theta_0$, than to demand $\rho \sim \rho_0$ … gives better result than earlier form.

Boussinesq approximation (2)

- Boussinesq - example

$$\frac{D\zeta'}{Dt} = \vec{k}\cdot\left(\frac{d\vec{V}}{dz}\times\nabla w'\right)$$

- In thunderstorms, derivation from the Boussinesq equation set describes growth of vorticity couplet relative to vertical shear vector



Notes