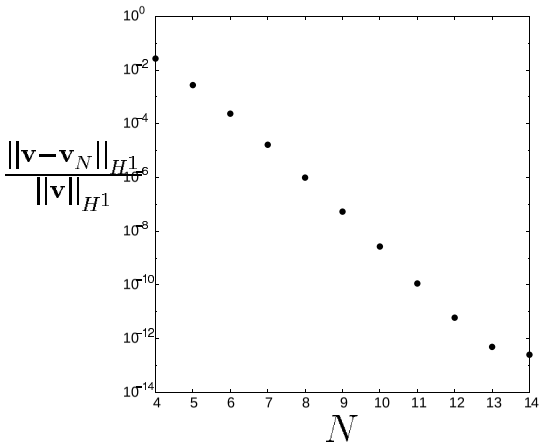
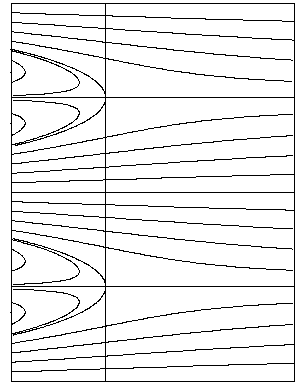
Background/History

- Outgrowth of Nekton 2.0 commercial code marketed by Fluent and developed by Rønquist, Ho, Fischer & Patera in 1986-1991, and modified by Fischer & Tufo in the '90s.
- Incompressible & unsteady Navier-Stokes with species transport.
- Variational-based spectral element formulation, similar to FEM.
- Elements are *locally* structured, *globally* unstructured.
- 2D, 3D, axisymmetric, with (some) moving mesh capability (Ho).
- Spectrally Accurate

Kovasznay Example

(*Proc. Roy. Soc., 1948*)





$$
\begin{aligned}
v_x &= 1 - e^{\lambda x}\cos 2\pi y \\
v_y &= \frac{\lambda}{2\pi} e^{\lambda x}\sin 2\pi y \\
\lambda &:= \frac{Re}{2} - \sqrt{\frac{Re^2}{4} + 4\pi^2}
\end{aligned}
$$

1D Convection Example

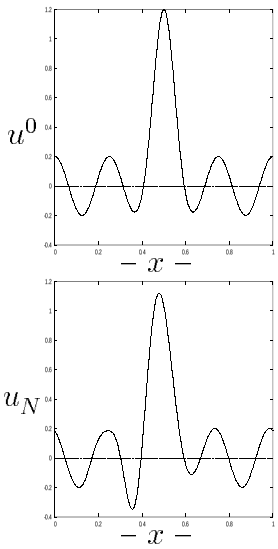
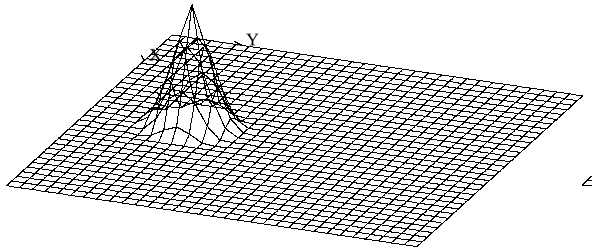


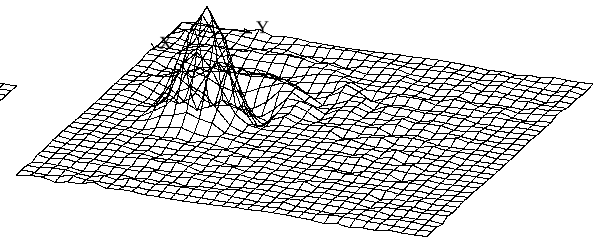
Table 1: Relative error at time $t = 10$, hyperbolic problem.

$\mathcal{N}$	Δt	$N = 1$	$N = 2$	$N = 4$	$N = 8$	$N = 16$	$N = 32$
64	.0025000	8.09e–1	1.29e–1	3.19e–2	2.91e–2	—	—
64	.0012500	8.13e–1	1.41e–1	1.27e–2	4.58e–3	4.11e–3	—
64	.0006250	8.13e–1	1.42e–1	1.22e–2	1.08e–3	5.43e–4	5.22e–4
64	.0003125	8.14e–1	1.43e–1	1.23e–2	8.27e–4	8.90e–5	6.55e–5
128	.0100000	—	—	—	—	—	—
128	.0012500	6.59e–1	1.42e–2	4.16e–3	4.10e–3	—	—
128	.0006250	6.60e–1	1.54e–2	6.14e–4	5.22e–4	5.22e–4	—
128	.0003125	6.60e–1	1.56e–2	2.00e–4	6.58e–5	6.55e–5	6.55e–5
256	.0025000	2.88e–1	—	—	—	—	—
256	.0012500	3.01e–1	4.66e–3	4.10e–3	—	—	—
256	.0006250	3.03e–1	1.51e–3	5.26e–4	5.22e–4	—	—
256	.0003125	3.03e–1	1.71e–3	7.02e–5	6.55e–5	6.55e–5	—

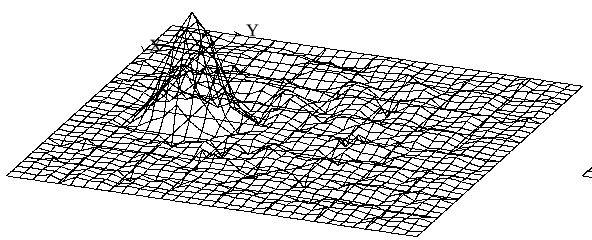
Numerical Dispersion vs. Order



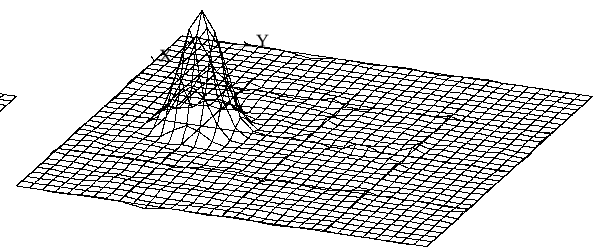
Initial Condition



$K_1 = 16,\ N = 2$



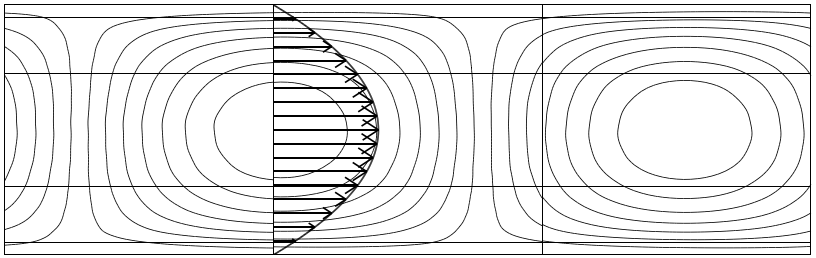
$K_1 = 8,\ N = 4$



$K_1 = 4,\ N = 8$

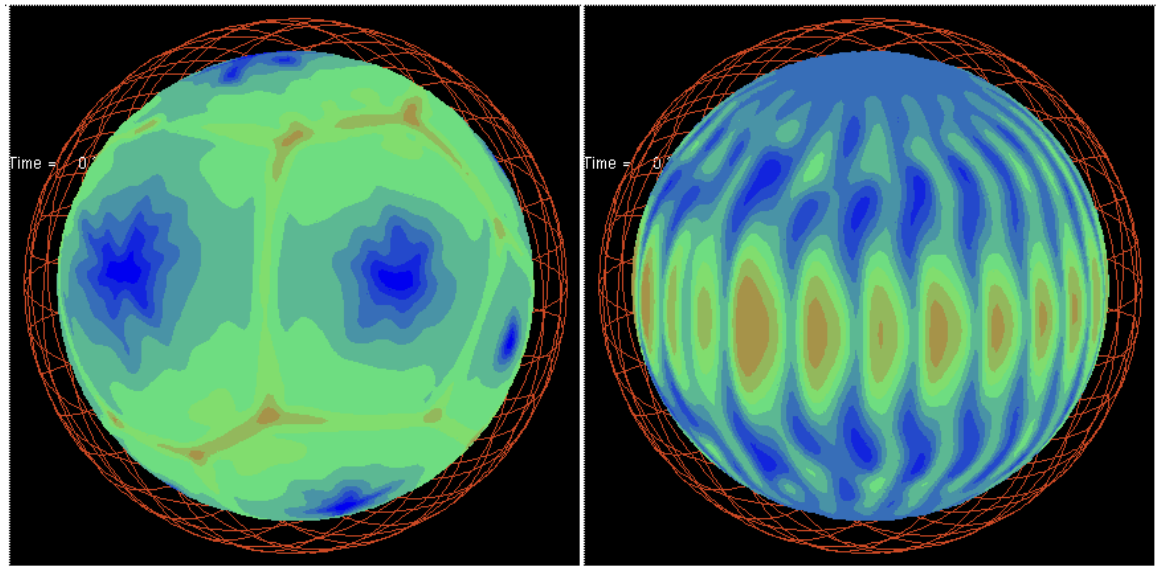
Error in Orr-Sommerfeld Growth Rates, $Re = 7500$

	$\Delta t = 0.003125$		$N = 17$	2nd Order		3rd Order	
N	$\alpha = 0.0$	$\alpha = 0.2$	Δt	$\alpha = 0.0$	$\alpha = 0.2$	$\alpha = 0.0$	$\alpha = 0.2$
7	0.23641	0.27450	0.20000	0.12621	0.12621	171.370	0.02066
9	0.00173	0.11929	0.10000	0.03465	0.03465	0.00267	0.00268
11	0.00455	0.01114	0.05000	0.00910	0.00911	161.134	0.00040
13	0.00004	0.00074	0.02500	0.00238	0.00238	1.04463	0.00012
15	0.00010	0.00017	0.01250	0.00065	0.00066	0.00008	0.00008



Convection in Deep Atmospheric Model

$Ra = 20,000$, increasing Ta



Standard Nek5000 Transport Equations

$$
\begin{aligned}
\rho\frac{D\mathbf{u}}{Dt} + \nabla p &= \nabla\cdot\mu\left(\nabla\mathbf{u}+\nabla^T\mathbf{u}\right) + \mathbf{f} \\
\nabla\cdot\mathbf{u} &= 0 \\
\rho c_p\frac{DT}{Dt} &= \nabla\cdot k\nabla T + q \\
\rho c_1\frac{D\Psi_1}{Dt} &= \nabla\cdot k_1\nabla\Psi_1 + q_1 \\
&\vdots
\end{aligned}
$$

- $\mathbf{f} = \mathbf{f}(t, \mathbf{x}, \mathbf{u}, T, \Psi_j, \ldots)$
- *Boussinesq*: $\mathbf{f} = \rho g\beta T\hat{\mathbf{z}},\ \beta := -\frac{1}{\rho}\frac{\partial\rho}{\partial T}\Big|_p,\ \ Ra = \frac{g\beta\Delta T L^3\rho_0^2}{k\mu}$.
- In principle, ρ can also be a function (though no longer I.N.S.)
- μ, k, k_j can also be functions.

User Input for Nek5000 Transport Equations

$$\texttt{utrans}\frac{D\Psi}{Dt} = \nabla \cdot \texttt{udiff}\nabla\Psi + \texttt{qvol}$$

```
      subroutine uservp (ix,iy,iz,ieg)
      include 'SIZE'
      include 'TOTAL'
      include 'NEKUSE'
c
      udiff =x+y+time
      utrans=1.
c
      return
      end
c-----------------------------------------------------------------------
      subroutine userq  (ix,iy,iz,ieg)
      include 'SIZE'
      include 'TOTAL'
      include 'NEKUSE'
c
      qvol   = sin(time)
c
      return
      end
```

Anelastic Models — *Simplified*

Lantz & Fan '99 – mixing length theory (*many* unspecified constants)

Background State:

$$\frac{dp_0}{dz} = -\rho_0 g$$

$$T_0 ds_0 = 0 \implies \frac{dT_0}{dz} = -\sigma \frac{\delta_p g}{c_p}$$

$$\delta_p := \frac{\partial \ln \rho}{\partial \ln T}$$

Actually use ($m = \frac{3}{2}$):

$$\rho_0 = \left[1 - \frac{z}{m+1}\right]^m \qquad (70)$$

$$T_0 = \left[1 - \frac{z}{m+1}\right] \qquad (71)$$

NOTE: ASH code does *not* assume isentropic background state.

Anelastic Models — LF I

Momentum:

$$\rho_0 \frac{D\mathbf{u}}{Dt} + \nabla p_1 = \frac{1}{Re} \nabla \cdot \mathbf{\Pi} + \rho_1 g \hat{\mathbf{z}} \tag{30}$$

$$\nabla \cdot \rho_0 \mathbf{u} = 0 \tag{33}$$

Entropy transport:

$$\rho_0 T_0 \frac{Ds_1}{Dt} = \frac{1}{Pe} \nabla \cdot K \rho_0 T_0 \nabla s_1 \tag{32}$$

E.O.S:

$$\longrightarrow \quad \rho_1(\rho_0, T_0, p_0, p_1)$$

Anelastic Models — LF II (M.L.T. + Ideal Gas)

Momentum:

$$\rho_0 \frac{D\mathbf{u}}{Dt} + \rho_0 \nabla \phi = \frac{1}{Re} \nabla \cdot \mathbf{\Pi} + \rho_0 g \frac{\delta_p}{c_p} s_1 \hat{\mathbf{z}} \tag{45}$$

$$\nabla \cdot \rho_0 \mathbf{u} = 0 \tag{33}$$

$$\phi := \frac{p_1}{\rho_0}$$

...plus entropy (s_1) transport (32).

- Very much like Boussinesq (from E.O.S. perspective).
- Strange multiplier in front of pressure term.

Standard Unsteady Stokes Solve

$$\begin{bmatrix} H & -D^T \\ -D & 0 \end{bmatrix} \begin{pmatrix} \underline{\mathbf{u}} \\ \underline{p} \end{pmatrix}^n = \begin{pmatrix} \underline{\mathbf{f}} \\ \underline{0} \end{pmatrix}$$

$H = \frac{\rho_0}{\Delta t} B + \mu A$, A – Laplacian, B – diagonal mass matrix $\underline{f}$ – nonlinear terms, etc.

Time splitting of discrete system *(Perot, JCP'93)*

$$\begin{bmatrix} H & -D^T \\ -D & 0 \end{bmatrix} \begin{pmatrix} \underline{\mathbf{u}} \\ \delta\underline{p} \end{pmatrix}^n = \begin{pmatrix} \underline{\mathbf{f}} + D^T \underline{p}^{n-1} \\ \underline{0} \end{pmatrix}$$

$$\begin{bmatrix} H & -HQD^T \\ -D & 0 \end{bmatrix} \begin{pmatrix} \underline{\mathbf{u}} \\ \delta\underline{p} \end{pmatrix}^n = \begin{pmatrix} \underline{\mathbf{f}} + D^T \underline{p}^{n-1} + (I - HQ) D^T \delta\underline{p} \\ \underline{0} \end{pmatrix}$$

Choose $Q = \left(\frac{\rho_0}{\Delta t} B\right)^{-1} \implies (I - HQ) = -\Delta t \, \nu \, AB^{-1}$.

Formal Block-Gaussian Elimination (Uzawa decoupling):

$$\begin{bmatrix} H & -HQD^T \\ 0 & E \end{bmatrix} \begin{pmatrix} \underline{\mathbf{u}} \\ \delta \underline{p} \end{pmatrix}^n = \begin{pmatrix} \underline{\mathbf{f}} + D^T \underline{p}^{n-1} \\ \underline{g} \end{pmatrix}$$

$E := D \left(\frac{\rho_0}{\Delta t} B \right)^{-1} D^T$ — SPD Schur complement for pressure.

LF-I Unsteady Stokes Solve

$$\begin{bmatrix} H & -D^T \\ -D\rho_0 & 0 \end{bmatrix} \begin{pmatrix} \underline{\mathbf{u}} \\ \underline{p} \end{pmatrix}^n = \begin{pmatrix} \underline{\mathbf{f}} \\ \underline{0} \end{pmatrix}$$

Splitting + Uzawa decoupling:

$$\begin{bmatrix} H & -HQD^T \\ 0 & E \end{bmatrix} \begin{pmatrix} \underline{\mathbf{u}} \\ \delta\underline{p} \end{pmatrix}^n = \begin{pmatrix} \underline{\mathbf{f}} + D^T\underline{p}^{n-1} \\ \underline{g} \end{pmatrix}$$

$E := D\rho_0 \left(\frac{\rho_0}{\Delta t}B\right)^{-1} D^T = \frac{1}{\Delta t}DB^{-1}D^T.$

E is a consistent Poisson operator.

LF-II Unsteady Stokes Solve

$$\begin{bmatrix} H & -\rho_0 D^T \\ -D\rho_0 & 0 \end{bmatrix} \begin{pmatrix} \underline{\mathbf{u}} \\ \underline{\phi} \end{pmatrix}^n = \begin{pmatrix} \underline{\mathbf{f}} \\ \underline{0} \end{pmatrix}$$

Splitting + Uzawa decoupling:

$$\begin{bmatrix} H & -HQD^T \\ 0 & E \end{bmatrix} \begin{pmatrix} \underline{\mathbf{u}} \\ \delta\underline{\phi} \end{pmatrix}^n = \begin{pmatrix} \underline{\mathbf{f}} + D^T \underline{p}^{n-1} \\ \underline{g} \end{pmatrix}$$

$E := D\rho_0 \left(\frac{1}{\Delta t} B\right)^{-1} D^T = \frac{1}{\Delta t} D\rho_0 B^{-1} D^T.$

Summary:

Std: $E = \frac{1}{\Delta t} D\rho_0^{-1} B^{-1} D^T$

LF-I: $E = \frac{1}{\Delta t} D B^{-1} D^T$

LF-II: $E = \frac{1}{\Delta t} D\rho_0 B^{-1} D^T$

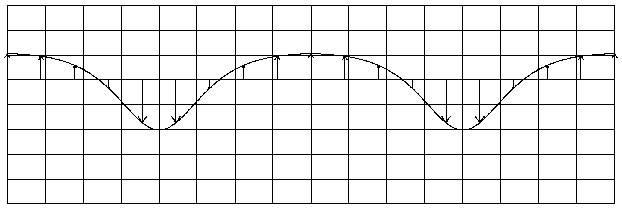
User Input for LF-II Nek5000 Transport Equations

```
      subroutine uservp (ix,iy,iz,ieg)
      include 'SIZE'
      include 'TOTAL'
      include 'NEKUSE'
c
      common /lantzfanc/ g,xi,gamma,cp,m
      real               g,xi,gamma,cp,m
      common /lantzfana/ rho1(lx1,ly1,lz1,lelt)
     $                 , rho0(lx1,ly1,lz1,lelt)
     $                 , T0  (lx1,ly1,lz1,lelt)
c
      visc = param(2)
      udiff =visc
      utrans=1.
      if (ifield.eq.2) then     ! Entropy transport
         ie      = gllel(ieg)
         conduct = param(8)
         utrans  = rho0(ix,iy,iz,ie)*t0(ix,iy,iz,ie)
         udiff   = conduct*rho0(ix,iy,iz,ie)*t0(ix,iy,iz,ie)  ! lack of better
      endif
c
      return
      end
```

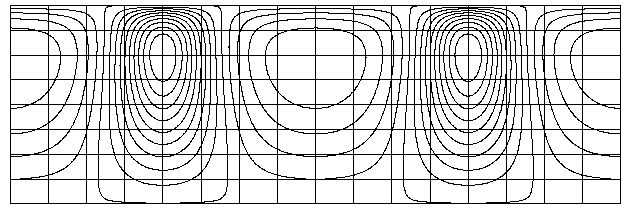
```
      subroutine userf  (ix,iy,iz,ieg)
      include 'SIZE'
      include 'TOTAL'
      include 'NEKUSE'
c
      common /lantzfanc/ g,xi,gamma,cp,m
      real               g,xi,gamma,cp,m
c
      ie = gllel(ieg)
      if (if3d) then
         ffx = 0.0
         ffy = 0.0
         ffz =  g*t(ix,iy,iz,ie,1)/cp
      elseif (ifaxis) then
         ffx = -g*t(ix,iy,iz,ie,1)/cp
         ffy = 0.0
         ffz = 0.0
      else
         ffx = 0.0
         ffy =  g*t(ix,iy,iz,ie,1)/cp
         ffz = 0.0
      endif
c
      return
      end
```

A Test Problem

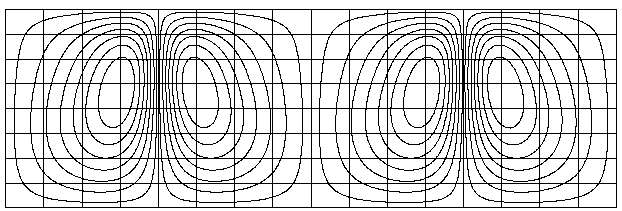
$Ra \approx 1000$, $h = 2H$



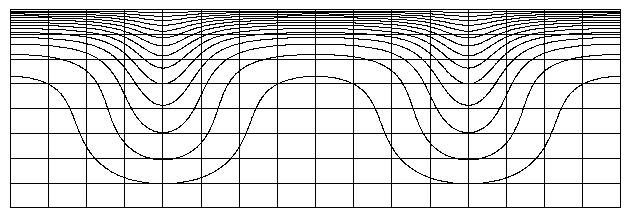
Vertical Velocity



Divergence



Vorticity



Entropy