Some aspects of the computation of the 3D normal-mode functions

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Outline

1. Normal mode software
   - developed as my work in MODES project
   - tutorial after this talk

2. -3 and -5/3 power spectra in zonal wavenumber domain
   - Rossby wave forms -3 power spectrum
   - Gravity wave forms -5/3 power spectrum

3. Vertical structure functions
   - -3 power law of kinetic energy spectrum in the vertical wavenumber domain

4. Toward high resolution computation with GPGPU
   - Fourier transform
   - Associated Legendre functions and Hough functions
3D Normal mode energetics

- A method to convert atmospheric variables in physical space to 3D spectral space.

<table>
<thead>
<tr>
<th>Basis functions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zonal</td>
</tr>
<tr>
<td>Meridional</td>
</tr>
<tr>
<td>Vertical</td>
</tr>
</tbody>
</table>

\[
\frac{\partial u}{\partial t} - 2\Omega \sin \theta v + \frac{1}{a \cos \theta} \frac{\partial \phi}{\partial \lambda} = -\nabla \cdot \nabla u - \omega \frac{\partial u}{\partial \sigma} + \frac{\tan \theta}{a} uu + F_u,
\]

\[
\frac{\partial v}{\partial t} + 2\Omega \sin \theta u + \frac{1}{a} \frac{\partial \phi}{\partial \theta} = -\nabla \cdot \nabla v - \omega \frac{\partial v}{\partial \sigma} - \frac{\tan \theta}{a} uu + F_v,
\]

\[
\frac{\partial c_p T}{\partial t} + \nabla \cdot \nabla c_p T + \omega \frac{\partial c_p T}{\partial \sigma} = \omega p_s \alpha + Q,
\]

\[
\frac{1}{a \cos \theta} \frac{\partial u}{\partial \lambda} + \frac{1}{a \cos \theta} \frac{\partial v \cos \theta}{\partial \theta} + \frac{\partial \omega}{\partial \sigma} = 0,
\]

\[
p_s \sigma \alpha = RT,
\]

\[
\frac{\partial \phi}{\partial \sigma} = -\frac{\alpha}{p_s}.
\]
Expanding to 3D normal mode space

Hough Functions can decompose the atmospheric state variables into Rossby mode and Gravity wave mode.

\[
\begin{align*}
\begin{pmatrix}
  u \\
  v \\
  \phi'
\end{pmatrix}
  &= \sum_i w_i \begin{pmatrix}
\sqrt{gh_i} & U_i \\
\sqrt{gh_i} & (-iV_i) \\
gh_i & Z_i
\end{pmatrix}
\end{align*}
\]

\[
\frac{dw_i}{d\tau} + i\sigma w_i = -i \sum_{j,k} r_{ijk} w_j w_k + f_i
\]

\[
E_i = \frac{1}{2} p_s h_m |w_i|^2
\]
1. Normal mode software
1. The code is Available from
   [http://www.fmf.uni-lj.si/~zagarn/modes.php](http://www.fmf.uni-lj.si/~zagarn/modes.php)
   - Serial execution
   - Including forward and backward transformation

2. Data format for input
   - GRIB1, GRIB2, binary, NetCDF

3. Required libraries
   - GRIB-API, NetCDF and Lapack should be installed

4. Vertical coordinate for input data
   - \( \sigma \)-coordinate, \( p \)-coordinate (not included released version), \( \sigma \)-\( p \) hybrid coordinate

5. Vertical structure functions
   - 3 type of solutions
     - Finite differential method
     - Spectral method (not included released version)
     - Analytical solution (not included released version)
6. Hough Functions

- based on the method by Paul N. Swarztrauber and Akira Kasahara (1985)
- fast computation
- difficulties in computing Hough functions when the equivalent height is small (less than 1m in my experience)
  - computational cost of Associated Legendre functions increases because the number of the grid of the ALFs is determined by the Lamb’s parameter \( \epsilon = 4\Omega^2 a^2/gh_m \)
- Dr. Tanaka’s method which solves the eigenvalue problem to obtain the Hough functions is stable. (not included in released version)

7. Fourier expansion

- FFTpack version 5.1 (by Paul N. Swarztrauber)

8. Not released version of the MODES software

- MPI-OpenMP hybrid code
- Using GPU (under developing)
2. -3 and -5/3 power spectra
(Terasaki et al., 2011)
Observation by aircraft

-3 power law in synoptic scale

-5/3 power law in meso-scale

Spectral slope shifts from -3 to -5/3 at wavelength below about 400km

Nastrom and Gage (1985)
JMA’s analysis (TL959L60)

Observation by aircraft

$k^{-3}$

$k^{-5/3}$

Nastrom and Gage (1985)

Zonal Energy Spectrum

Total = Rossby + Gravity

$-3$

$-5/3$

Nastrom and Gage (1985)

Terasaki, et al., (2011)
Results show that the total energy spectrum does not clearly represent the transition of the energy slope, but the total energy spectrum shifts from $k^{-3}$ to $k^{-5/3}$ gradually. The energy level of Rossby waves is higher in the synoptic scale, and that of gravity waves becomes higher in the mesoscale. It is found in this study that the energy spectra for Rossby and gravity modes cross each other around $k = 80$. It is essential for understanding these power laws in the general circulation that the energy spectra of Rossby and gravity waves obey the $k^{-3}$ and $k^{-5/3}$ laws, respectively. The schematic diagram of energy spectrum is shown in Fig. 4.

The ratio of Rossby wave energy to gravity wave energy clearly explains why the total energy shows the gradual spectral shift. The result of this study may indicate that the shifting wave number from $k^{-3}$ to $k^{-5/3}$ is determined just as a crossing wavenumber of Rossby wave and gravity wave spectra.

Terasaki et al. (2009) found that the energy spectrum of the vertical motion becomes white noise using NICAM experiment (3.5 km horizontal grid spacing), which has almost the same energy level at any horizontal scales. It is suggested that the $k^{-5/3}$ power spectral law in stratified turbulence may be explained by the saturation theory of the vertical motion. It is desired to examine the formation mechanism of energy spectrum in 3D normal mode energetics, and also to investigate the spectra with the high resolution model.

Fig. 2. The ratio of energy of the Rossby mode to gravity mode in Fig. 1.

Fig. 3. The energy spectrum for the barotropic mode as a function of dimensionless phase speed of the Rossby mode $c$. Energy levels are connected by dotted lines for the same zonal wavenumber $k$ with different meridional mode numbers $l$. The spectrum of $E = mc^2$ is drawn by solid line, where $m$ means a total mass of the atmosphere for unit area. The units of energy are J m$^{-1}$.

Fig. 4. Schematic diagram of energy spectrum for baroclinic atmosphere. The dotted and dashed lines show the energy spectra for Rossby and gravity modes, respectively. The solid line shows the total (Rossby + gravity) energy spectrum.

Rossby mode => -3 power law

Gravity mode => -5/3 power law

Energy slope changes from -3 power law to -5/3 power law gradually.

Dr. Ofuchi decomposed the horizontal wind into rotational and divergent winds, but he could not find such spectral transition. (personal communication)
3. Vertical structure functions

numerical and analytical solutions
(Terasaki and Tanaka, 2007)
Vertical structure functions

Vertical structure equation

\[ \frac{\partial}{\partial \sigma} \left( \sigma^2 \frac{\partial G_m}{\partial \sigma} \right) + \frac{R \gamma}{gh_m} G_m = 0 \]

\begin{align*}
\text{m:} & \quad \text{vertical mode} \\
\text{G}_m: & \quad \text{vertical structure function} \\
\text{R:} & \quad \text{Gas constant} \\
\text{h}_m: & \quad \text{equivalent depth (m)} \\
\gamma: & \quad \text{static stability parameter (K)}
\end{align*}

Discretize the equation and solve the eigenvalue problem

Global mean temperature profile is only input data
Numerical solutions

JRA-25: 23 vertical layers

Large aliasing in higher vertical modes
Global averaged energy spectra have large aliasing in higher vertical modes.
Vertical structure functions

Vertical structure equation

\[
\frac{\partial}{\partial \sigma} \left( \sigma^2 \frac{\partial G_m}{\partial \sigma} \right) + \frac{R \gamma}{g h_m} G_m = 0
\]

- \( G_m \): vertical structure function
- \( R \): Gas constant
- \( h_m \): equivalent depth (m)
- \( \gamma \): static stability parameter

\[
\gamma = \frac{RT_0}{c_p} - \sigma \frac{dT_0}{d\sigma} = \text{const}
\]

Euler Equation

Barotropic component \((m=0)\)

\[
G_0(\sigma) = C_1 \sigma^{r_1} + C_2 \sigma^{r_2}
\]

Baroclinic component \((m>0)\)

\[
G_m(\sigma) = \sigma^{\frac{1}{2}} \{ C_1 \cos(\mu_m \ln \sigma) + C_2 \sin(\mu_m \ln \sigma) \}
\]
Analytical vertical structure functions
Energy spectrum in vertical wavenumber domain

- There are two clear peaks, one is in the barotropic component, and the other is in \( m=4 \) (corresponding to \( h=250m \)).

- The kinetic energy spectrum in the vertical wavenumber domain clearly shows \(-3\) power law using analytically derived vertical structure functions.
3. Very high resolution 3D normal mode energetics with GPGPU
Computational cost in 3D NMF

➢ Vertical direction • • • Vertical structure functions
   Eigenvalue problem for square matrix with number of vertical grid. The computational cost is very small.

➢ Zonal direction • • • Fourier expansion (cuFFT)
   Computational cost of Fourier transform is $O(N^2)$, but it can be reduced to $O(N\log N)$ by Fast Fourier transform.

➢ Meridional direction • • • Hough functions
   Large computational cost for
   • associate Legendre functions
   • solving eigenvalue problem ($O(N^3)$)
Associate Legendre Functions

**Associate Legendre Equation**

\[
(1-x^2) \frac{d^2y}{dx^2} - 2x \frac{dy}{dx} + \left\{ n(n+1) - \frac{m^2}{1-x^2} \right\} y = 0
\]

**Associate Legendre Functions**

\[
P_l^m(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} (P_l(x))
\]

\[
P_l^0(x) = (P_l(x))
\]

**Recurrence formula**

\[
(l-m+1)P_{l+1}^m(x) = (2l+1)xP_l^m(x) - (l+m)P_{l-1}^m(x)
\]

\[
2mxP_l^m(x) = -\sqrt{1-x^2} \left[ P_l^{m+1}(x) + (l+m)(l-m+1)P_l^{m-1}(x) \right]
\]
Associate Legendre Functions

Recurrence formula

\[(l - m + 1)P_{l+1}^m(x) = (2l + 1)xP_l^m(x) - (l + m)P_{l-1}^m(x)\]

\[2mxP_l^m(x) = -\sqrt{1 - x^2}\left[P_{l+1}^m(x) + (l + m)(l - m + 1)P_{l-1}^m(x)\right]\]

Advantage

- Computational cost is low

Disadvantage

- Overflow occurs when the order increases.
- Accumulated roundness error affects the high order computations of the ALFs.
Associate Legendre Functions

- Yu et al. (2012)

Integral method is used to avoid the problems with recurrence formula

When I-m is even number

$$P_l^m(x) = \frac{1}{\pi} \frac{2n+1}{P_l^m(0)} \int_0^{\pi/2} P_l(\sqrt{1-x^2} \cos \lambda) \cos m\lambda d\lambda$$

When I-m is odd number

$$P_l^m(x) = \frac{\sqrt{1-x^2}}{x} \left[ \frac{\sqrt{(1+\delta_{l,m})(n-m+1)(n+m)}}{2m} \times P_l^{m-1} ight. \\
+ \left. \frac{\sqrt{(n+m-1)(n-m)}}{2m} \times P_l^{m+1} \right]$$

Computational cost is much higher than recurrence method. $O(N^4)$ of computational cost is required for integral method. The computation of Legendre functions is hotspot in this method.
Elapse time (1 node)

- HA-PACS in University of Tsukuba
  - 16 CPU cores / node
  - 4GPUs (Tesla M2090) / node
- Compare the elapse time using 1 node
- Computational cost is proportional to $O(N^4)$ (if $N$ becomes 2x, computational cost becomes 16x)

<table>
<thead>
<tr>
<th>N</th>
<th>1MPI 1openmp</th>
<th>1MPI 16openmp</th>
<th>1MPI 16openmp + 1GPU</th>
<th>1MPI 16openmp + 4GPU</th>
</tr>
</thead>
<tbody>
<tr>
<td>512</td>
<td>3419.9 (s)</td>
<td>225.8 (s)</td>
<td>32.5 (s)</td>
<td>10.4 (s)</td>
</tr>
<tr>
<td>1024</td>
<td>×</td>
<td>3562.6 (s)</td>
<td>643.9 (s)</td>
<td>186.7 (s)</td>
</tr>
<tr>
<td>2048</td>
<td>×</td>
<td>×</td>
<td>10281.5 (s)</td>
<td>3026.6 (s)</td>
</tr>
</tbody>
</table>

×: give up computing
Scalability test

![Scalability Test Graph]

The graph shows the elapsed time (in seconds) for different numbers of nodes. The data points are as follows:

<table>
<thead>
<tr>
<th># of nodes</th>
<th>1 node</th>
<th>2 nodes</th>
<th>4 nodes</th>
<th>8 nodes</th>
<th>16 nodes</th>
</tr>
</thead>
<tbody>
<tr>
<td>2048</td>
<td>3026.6 (s)</td>
<td>1516.2 (s)</td>
<td>765.1 (s)</td>
<td>384.4 (s)</td>
<td>200.2 (s)</td>
</tr>
<tr>
<td>5120</td>
<td>11636.2 (s)</td>
<td></td>
<td></td>
<td></td>
<td></td>
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</tbody>
</table>
Summary

✓ Software of the Normal mode Energetics was developed in MODES project.
  Download from http://www.fmf.uni-lj.si/~zagarn/modes.php

✓ Vertical structure functions
  • It is found that kinetic energy spectrum in the vertical wavenumber domain
    obeys -3 power law by using analytical vertical structure functions.

✓ -3 and -5/3 power spectra in normal mode space
  • Rossby wave forms -3 power spectrum
  • Gravity wave forms -5/3 power spectrum

✓ Toward high resolution computation with GPGPU
  • Computational cost and accuracy of the Associated Legendre functions are
    very important.
  • Integral method can compute them very accurately, but computational cost
    is very high.