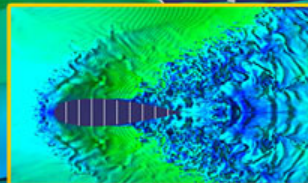
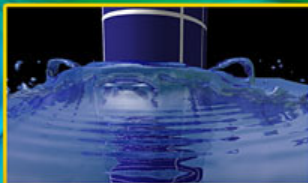
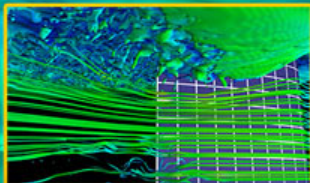


Numerical Fluid Dynamics

0 1.4 2.8
Normalized Velocity

daac.hpc.mil/gallery/



Dr. Douglas Dommermuth, Mr. Donald Wyatt, Mr. Scott Graham
Mr. John Kuhn, Mr. Thomas O'Shea and Dr. Tricia Sur
"Large-Eddy Simulation of Steep Breaking Waves and Thin Spray Sheets around a Ship"

NFA: A Cartesian-grid and volume-of-fluid formulation for simulating breaking waves around ships including spray formation and air entrainment. ONR Program Manager: Dr. Patrick Purtell. Challenge Project Manager: Dr. Ki-Han Kim. ONR contract number: N00014-02-C-0017

DAAC
Data Analysis and Assessment Center

CLASS 15 - TUE., MAR. 5, 2019

ATMS 502
CSE 566

Tuesday,
5 March 2019

Class #15

- Pgm3 due Thu Mar. 7

Plan for Today

- **1) Space differencing**
 - Differential-difference approach
 - Phase speed & group velocity
 - Impacts of higher order, added diffusion
- **2) Programming input/output**
 - C and Fortran considerations
- **3) Program 4: *continued***
 - Nest placement / movement
- **4) Skamarock & Klemp**
 - Global/local refinement
 - A full AMR method, explained

Space differencing

3

Reference pages for this section:

- Durran (2010) § 3.3, p. 100+
- C008 – Truncation error
- C009 – Resolution
- C010 – AMR / nesting
- C051 – Nesting: grid placement, movement

Review: Poorly resolved waves

4

- Centered schemes preserve **amplitude** of Fourier components, but **dispersion** yields numerical dissipation in solution
- “Almost all finite difference schemes **fail to propagate** the $2\Delta x$ wave.
- Negative **group velocities** for $2\Delta x$ waves
- Higher accuracy does **not** help with poorly-resolved waves.

Overview: Space differencing

5

- Task: Isolate *just* the spatial errors
 - differential-difference equation
 - ✦ leave time derivative: as a derivative
 - ✦ apply differencing to spatial derivative
 - ✦ insert complex exponential involving time
 - ✦ simplify to obtain frequency
 - computing phase speed
 - ✦ frequency divided by wavenumber
 - ✦ if phase speed depends on k : dispersive.
 - if this was a linear, constant speed problem, wavenumber dependence $c(k)$ represents *numerical error*.
 - compute group velocity
 - ✦ derivative of frequency w.r.t. wavenumber

Space Differencing

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- *How to address space/time differencing separately?*

- Space: *differential-difference equations*

- ✦ Wherein we say: what time differencing?

- ✦ Let's look at just *2nd-order centered space*

$$\frac{du_j}{dt} + c \left(\frac{u_{j+1} - u_{j-1}}{2\Delta x} \right) = 0 \quad \bullet \text{ no } n+1, n... \text{ superscripts}$$

- ✦ And we substitute a slightly different form:

$$u_j(t) = e^{i(kj\Delta x - \omega_{2c}t)}$$

- ✦ Key point: frequency ω can still be complex!!

- Why is this important? (we'll discuss this further, later)

Space Differencing

7

- Frequency eqn for 2nd-order ctr space

$$\frac{du_j}{dt} + c \left(\frac{u_{j+1} - u_{j-1}}{2\Delta x} \right) = 0 \quad \text{substitute: } u_j(t) = e^{i(kj\Delta x - \omega_{2c}t)}$$

- We get frequency equation:

$$-i\omega_{2c} u = -\frac{c}{2\Delta x} (e^{ik\Delta x} - e^{-ik\Delta x}) u \Rightarrow \omega = \frac{c \sin \beta}{\Delta x}$$

Real frequency: no amplitude error.
See Durran § 3.3.1

- Is this dispersive? Yes. $c(k)$!

$$c_{2c} = \frac{\omega}{k} = \frac{c \sin \beta}{k\Delta x}; \text{ for small } k\Delta x, c_{2c} \approx c \left(1 - \frac{\beta^2}{6} \right)$$

Note $\beta \rightarrow 0$ case

Space Differencing

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- Our expression for the *phase speed*:

$$c_{2c} = \frac{\omega}{k} = \frac{c \sin \beta}{k \Delta x}; \text{ for small } k \Delta x, c_{2c} \approx c \left(1 - \frac{\beta^2}{6} \right)$$

- *Lagging phase error. Note $c_{2c}(2\Delta x) = 0!$*

- *Group velocity*:

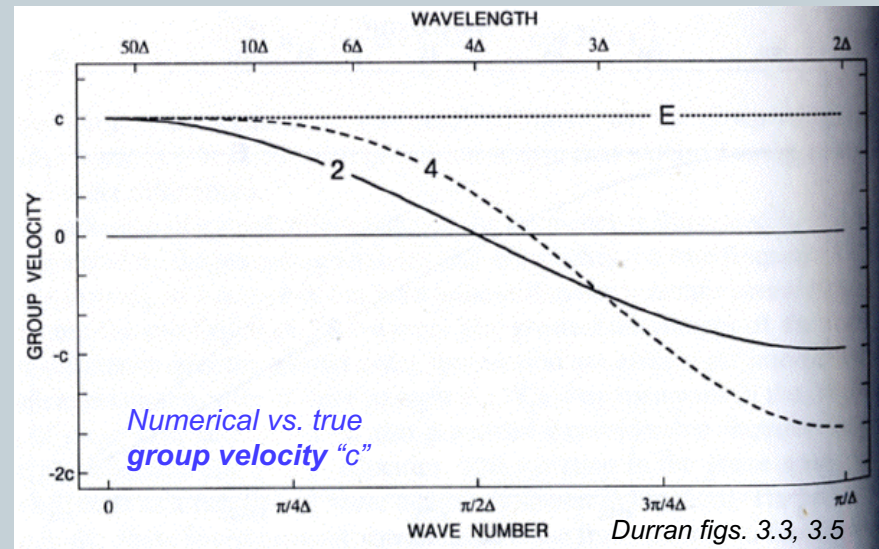
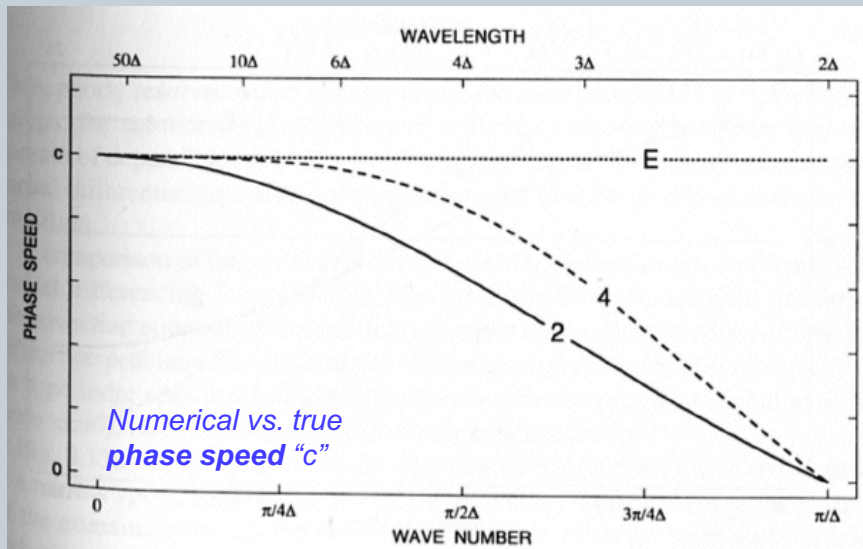
$$c_{g2c} = \frac{\partial \omega}{\partial k} = \frac{\partial}{\partial k} \left(\frac{c \sin \beta}{\Delta x} \right) = c (\cos \beta)$$

- *good for small β (long waves);*
- *terrible for small waves!! (why?)*

2nd vs. 4th order space diff.

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- *Summary: 2nd-order centered space differencing*

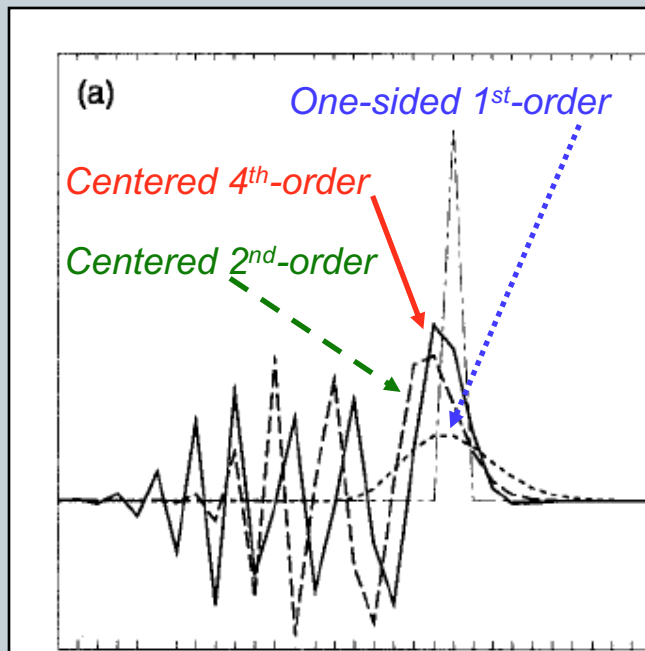


- **Phase speed** (left), **group velocity** (right)
- **Second order** (solid), **4th order** (dashed)
- **4th** better at "intermediate" wavelengths

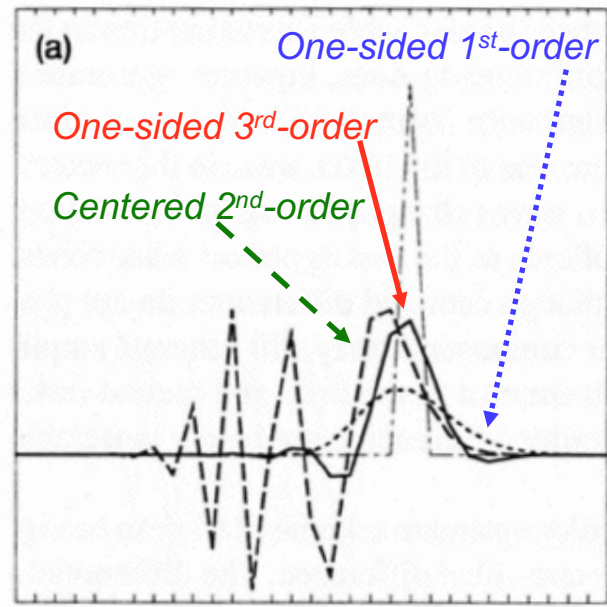
1st - 4th order space differencing

10

- *Higher centered vs. odd-ordered schemes*



*1-sided 1st order vs.
centered 2nd,4th*

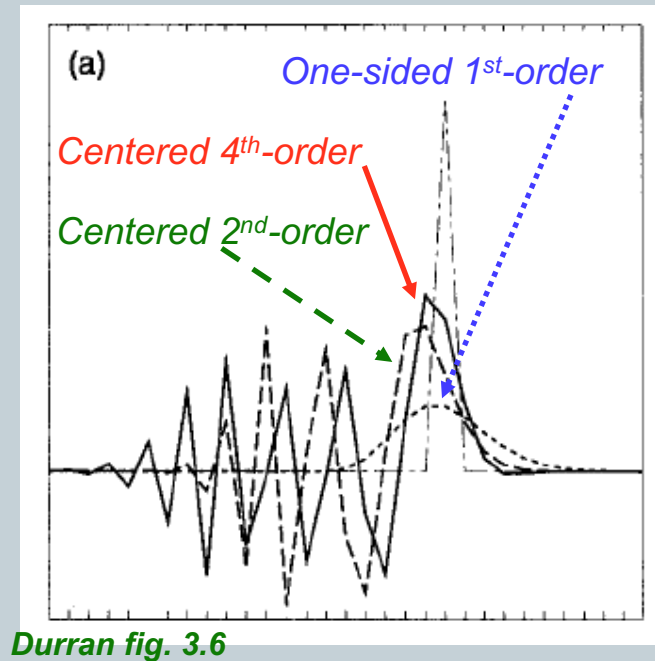


*1-sided 1st, 3rd order vs.
centered 2nd*

Distortion of the solution

11

- “**Centered schemes preserve the amplitude** of each individual Fourier component, [but] the various *components propagate at different speeds*, and thus the **superposition of these components ceases to properly represent the true solution**”
 - *Durran pp. 106-107*
 - With phase errors, wavelengths interfere – causing amplitude errors

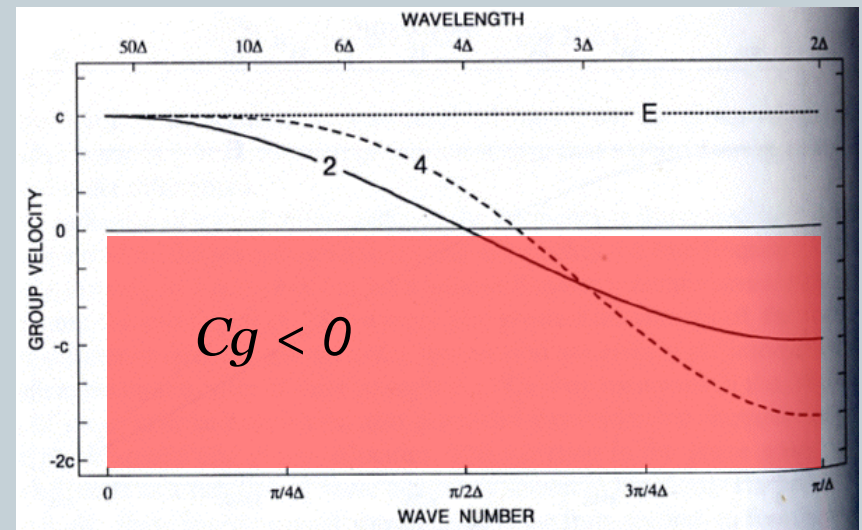


Group velocities

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- “In the *absence of dissipation* the large negative group velocities associated with the $2\Delta x$ wave rapidly spread short wavelength noise away from regions where $2\Delta x$ waves are forced.”

- *Durran pp. 106-107*



Group velocities

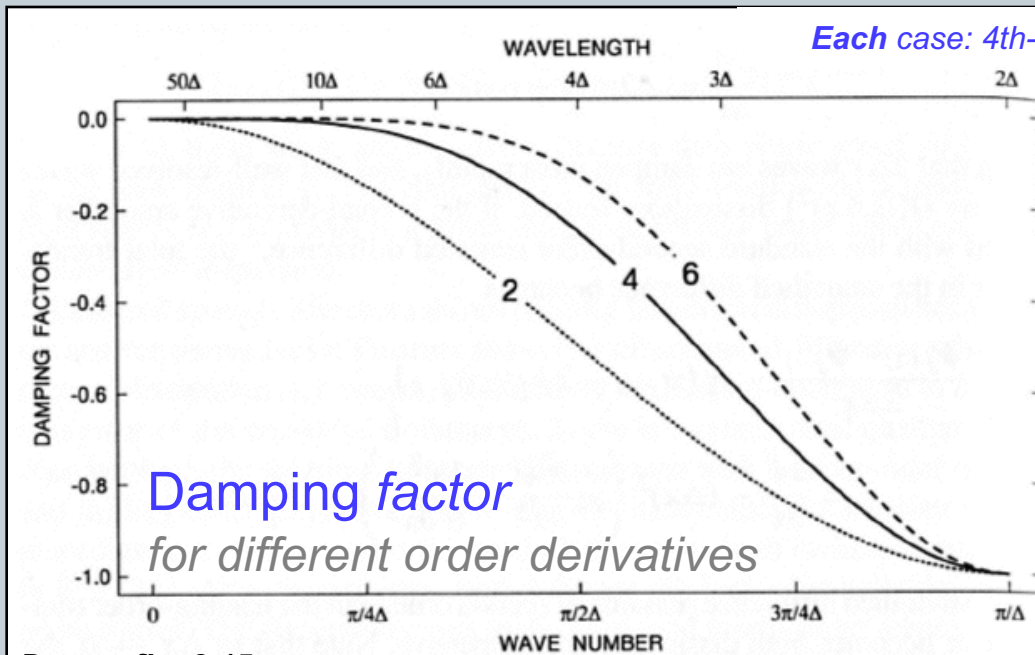
13

- “The **upstream propagation** of the $2\Delta x$ wave [is worse with 4th order than 2nd].
- “**Switching to a higher-order scheme does **not** improve the performance of finite-difference methods *when they are used to model poorly resolved features* like the spike ... in many respects the **4th-order solution is worse** than the 2nd-order result.**
- *Durran pp. 106-107*

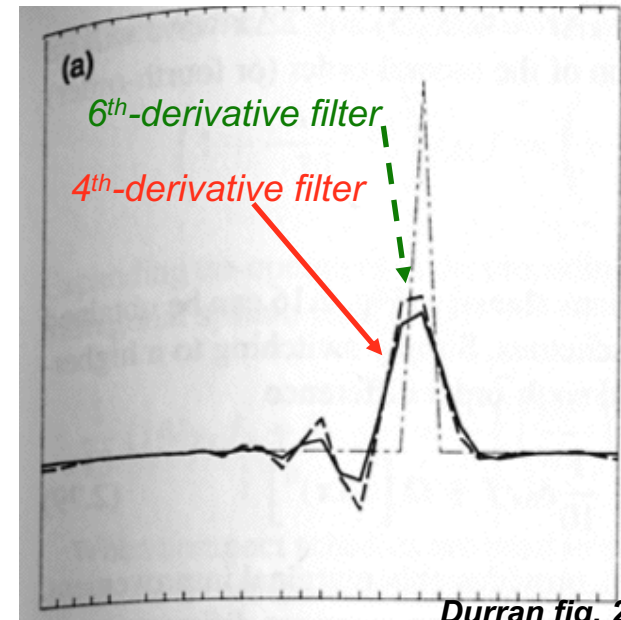
Explicit Artificial Dissipation

14

- *Added explicit damping can be beneficial*



Durran fig. 2.15



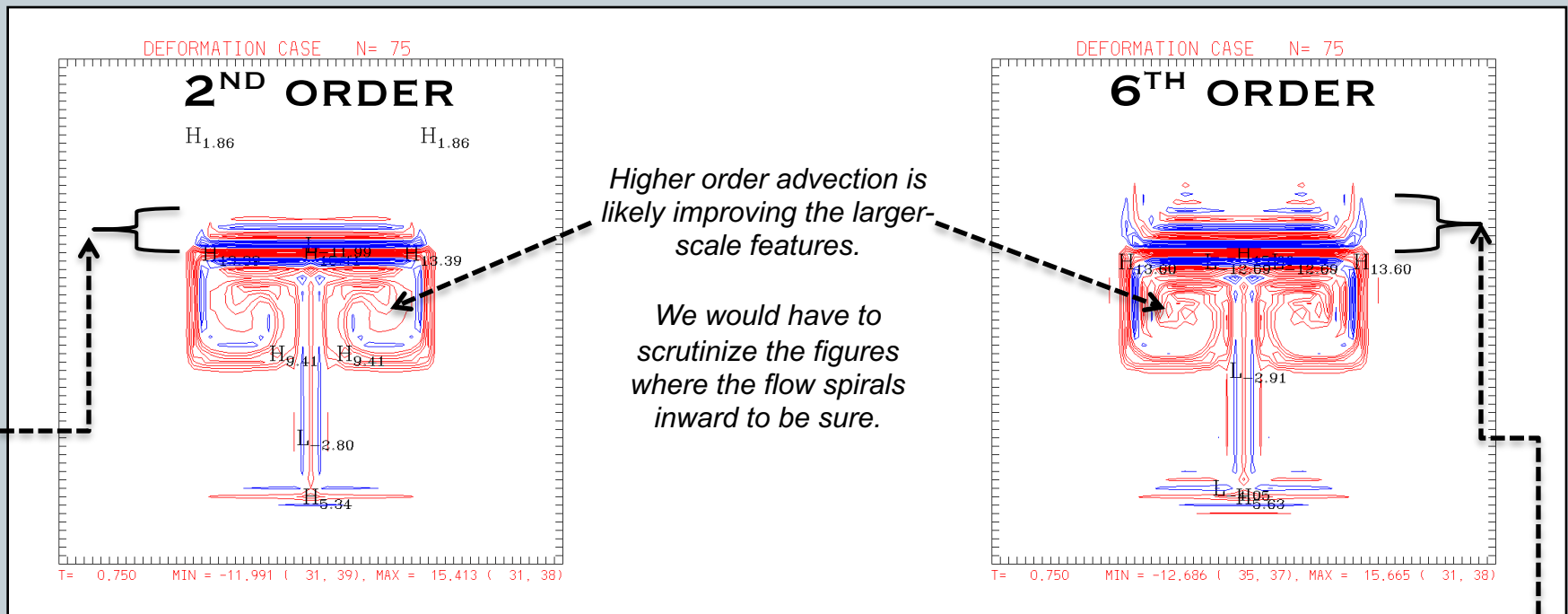
Durran fig. 2.16

Without filtering, errors w/dispersion of poorly-resolved Fourier components propagate without damping. Explicit diffusion reduces amplitude of these short waves.

Review: Added Dissipation

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- No damping here; just deformational flow tests with 2nd order (Lax-Wendroff) and 6th-order (Crowley) advection.



But notice the packing of contours at the top. This appears **worse** for 6th order, and probably represents greater dispersion in the region of sharpest gradients, in the deformational flow near the top of each figure.

Programming input/output

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To learn more:

- **web-search for**
 - *Linux I/O redirect*
 - *[Fortran or C] I/O*
 - *XML programming [Fortran or C]*
 - *NetCDF example [Fortran or C] or [go here](#)*

Linux I/O

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- Three classes of I/O, and ways to *redirect* I/O:
 - **stdin**: standard input
 - ✦ Fortran: *read*,nplot* or *read(5,*) nplot*
 - ✦ C: *scanf("%d",&nplot);*
 - ✦ Linux shell: *program < filename*
 - **stdout**: standard output
 - ✦ Fortran: *print*,nplot* or *write(6,*) nplot*
 - ✦ C: *printf("%d", nplot);*
 - ✦ Linux shell: *program > filename* or *program >> appendFile*
 - ✦ Linux shell, in+out: *program < inputFile > outputFile*
 - **stderr**: standard error
 - ✦ stderr: the *other* output stream ...
 - ✦ this can also be *redirected*.
 - ✦ the syntax depends on your command interpreter (shell).
 - C-shell & *tcsh*: redirect *both* stdout, stderr with: *program >& file*
 - Bash: redirect *both* stdout, stderr with: *program > file 2>&1*

A short script to run your program

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- So are you **tired** of this yet?

- login2% `pgm2`

- `360`

- `.075`

- `5`

- `y`

- So much better to run your program with the input specified directly in a script.

- See example at right!

- Good resource to get answers to your programming questions:

- stackoverflow.com

- In a *tcsh* or *bash* script:

```
#!/bin/tcsh or #!/bin/bash  
pgm2 << EOF
```

```
360
```

```
.075
```

```
5
```

```
y
```

```
1
```

```
...
```

```
EOF
```

EOF is a common LINUX abbreviation, short for "End of File". Really any word will work here!!

```
pgm2 << SickOfPgm2
```

```
...
```

```
SickOfPgm2
```

- Don't forget to make the script **executable**

```
chmod u+x myscript
```

- adds **execute** permission for the **user** (you).

Fortran and C: read/write text to file

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Fortran

- **read** from file directly:

```
open(1,file='filename', &
      status='old')
read(1,*) nplot
read(1,*) morestuff
close(1)
```

- **write** to file directly:

```
open(1,file='newfile', &
      status='unknown')
rewind(1)
write(1,*) nplot
close(1)
```

C

- **read** from file directly:

```
#include <stdio.h>
FILE *fp,*fopen();
fp=fopen("filename","r");
fscanf(fp,"%d", &nplot);
fclose(fp);
```

- **write** to file directly:

```
#include <stdio.h>
FILE *fp,*fopen();
fp=fopen("newfile","w");
fprintf(fp,"%d", nplot);
fclose(fp);
```

Fortran input via a *namelist*

20

- The code looks like:

```
namelist /namelist_name/ variable1, variable2, variable3 ...
```

! ... you still have to declare all these variable types!

```
open(1,file='namelist_filename',status='old')
```

```
read(1, NML=namelist_name)
```

```
close(1)
```

- The namelist file looks like:

```
&namelist_name
```

```
variable1 = -12.45,
```

```
variable2 = 73.123,
```

```
variable3 = .true.,
```

```
/
```

Reading and writing *XML*

21

- XML – eXtensible Markup Language

- designed to carry data.
- example at right

```
<?xml version="1.0"?>
<p5input>
  <dt> 0.5</dt>
  <dx>100</dx>
</p5input>
```

- For Fortran: *not really supported, but try these:*

- <http://xml-fortran.sourceforge.net>
- <http://homepages.see.leeds.ac.uk/~earawa/FoX/>
- <https://www.sciencedirect.com/science/article/pii/S235271101630036X>

- For C:

- Google “C xml parser library” : code.google.com/p/libroxml
- Gnome xml C parser, libxml : xmlsoft.org; also, wikipedia
- <https://stackoverflow.com/questions/9387610/what-xml-parser-should-i-use-in-c>

Reading and writing *NetCDF*

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- NetCDF is a data format with C and Fortran *APIs*
 - an API is *an Application Program Interface*
 - ✦ "*a set of routines, protocols and tools for building software applications. An API specifies how software components interact*" - [webopedia](#)
- NetCDF data has *your* data but also *metadata*
 - *metadata* is a set of data that describes and gives information about other data (*google*)
 - so your file could contain your array dimensions, field names, field *units*, and of course the data itself.
- Learn more here:
 - <https://www.unidata.ucar.edu/software/netcdf/examples/programs/>

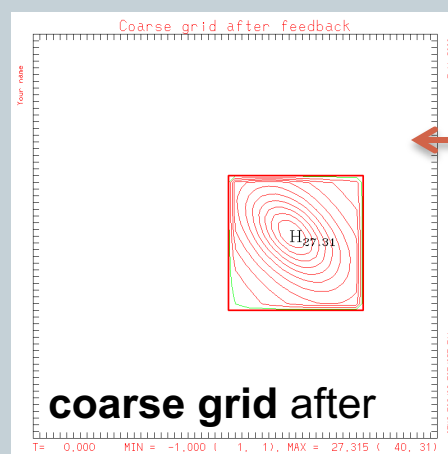
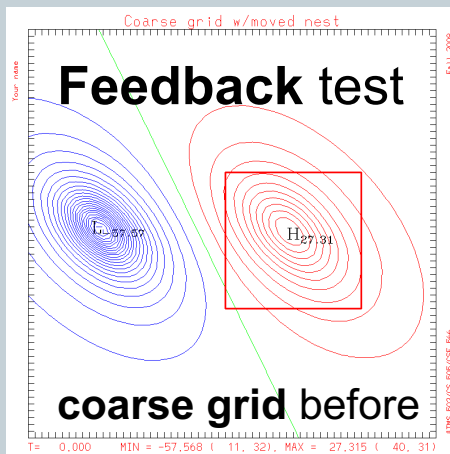
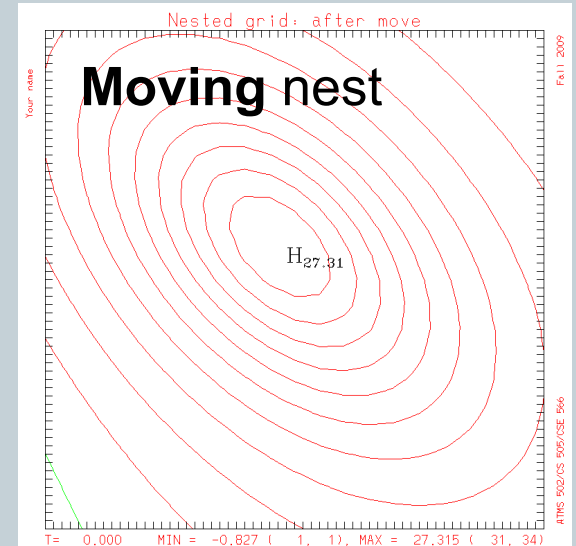
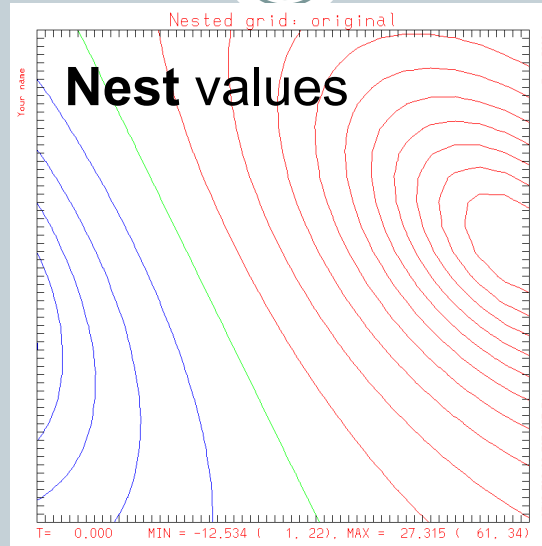
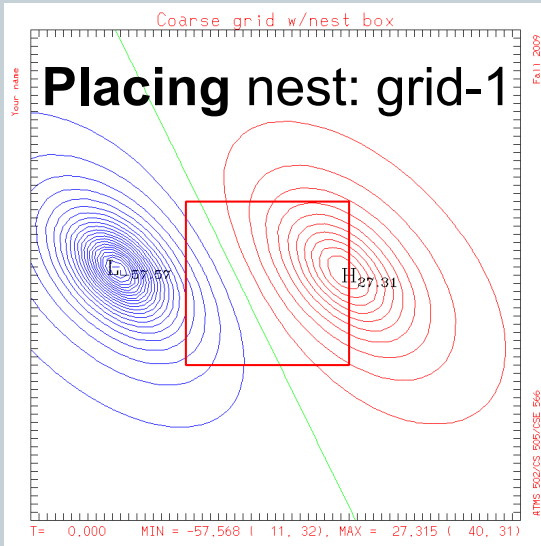
Program 4

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NEST PLACEMENT ALGORITHM

Review: Nesting routines

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Result *after* I set coarse grid to -1 everywhere, and then did **feedback**.

Determining the nest location (1)

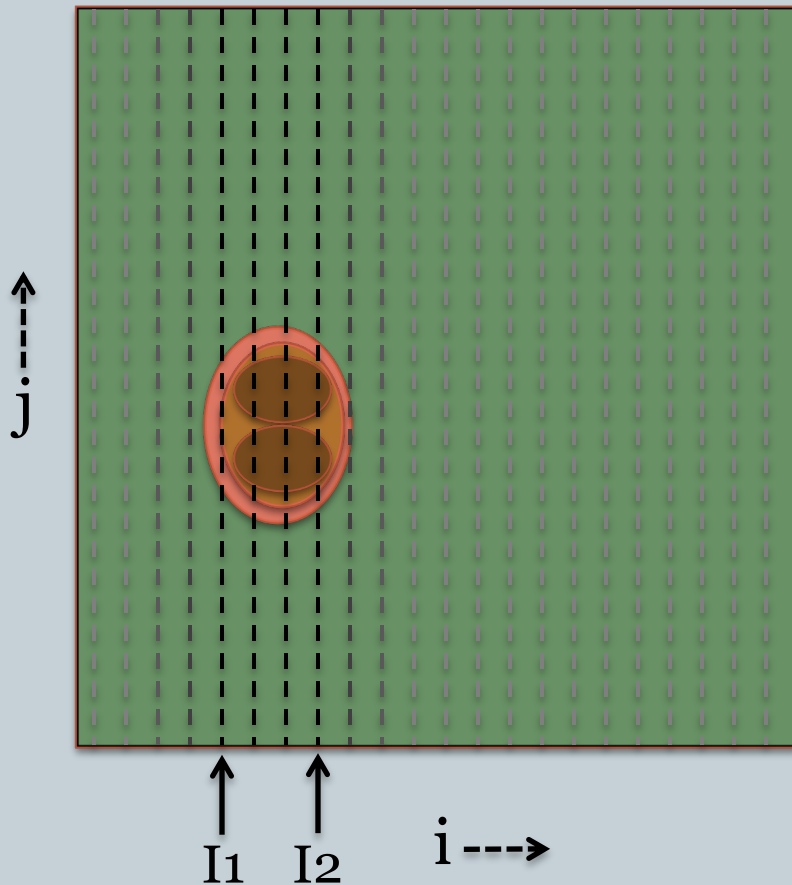
25

- Compute the 2-D truncation error (*T.E.*)
 - Done *consistent with 1-D directional splitting*; estimates T.E. from the max of the absolute value in the X- and Y-directions
- Locating the nest (*position on coarse grid*)
 - Set T.E. *threshold* as 50% of max T.E. over the 2-D T.E. array
 - “**Search**” inward from left, right, top, bottom edges, noting the I,J bounds at which you first find T.E. \geq the *threshold* value.
 - Nest *center* = integer, truncated value: $(I_1+I_2)/2$, $(J_1+J_2)/2$
 - Nest *size* = $(NX-1)/\text{refinement_ratio}$
 - $\text{NestX1} = I_{\text{center}} - \text{nestsize}/2$; $\text{NestX2} = \text{NestX1} + \text{nestsize}$
 - $\text{NestY1} = J_{\text{center}} - \text{nestsize}/2$; $\text{NestY2} = \text{NestY1} + \text{nestsize}$
 - **Check** if nest runs off coarse grid edge; fix if so.

Determining the nest location (2)

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Cartoon of T.E. on coarse grid.



- Example of finding left, right edges of T.E. region
 - For each i column, left to right ... check $TE(i,j)$ for all j rows – determine max value
 - Find first and last column (i) for which $\max \geq \text{threshold}$.
- Do same for top/bottom.
- Average I_1, I_2, J_1, J_2 for nest *center*. Nest *edges* depend on nest *size*.

Skamarock & Klemp

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ADAPTIVE MESH REFINEMENT PAPER

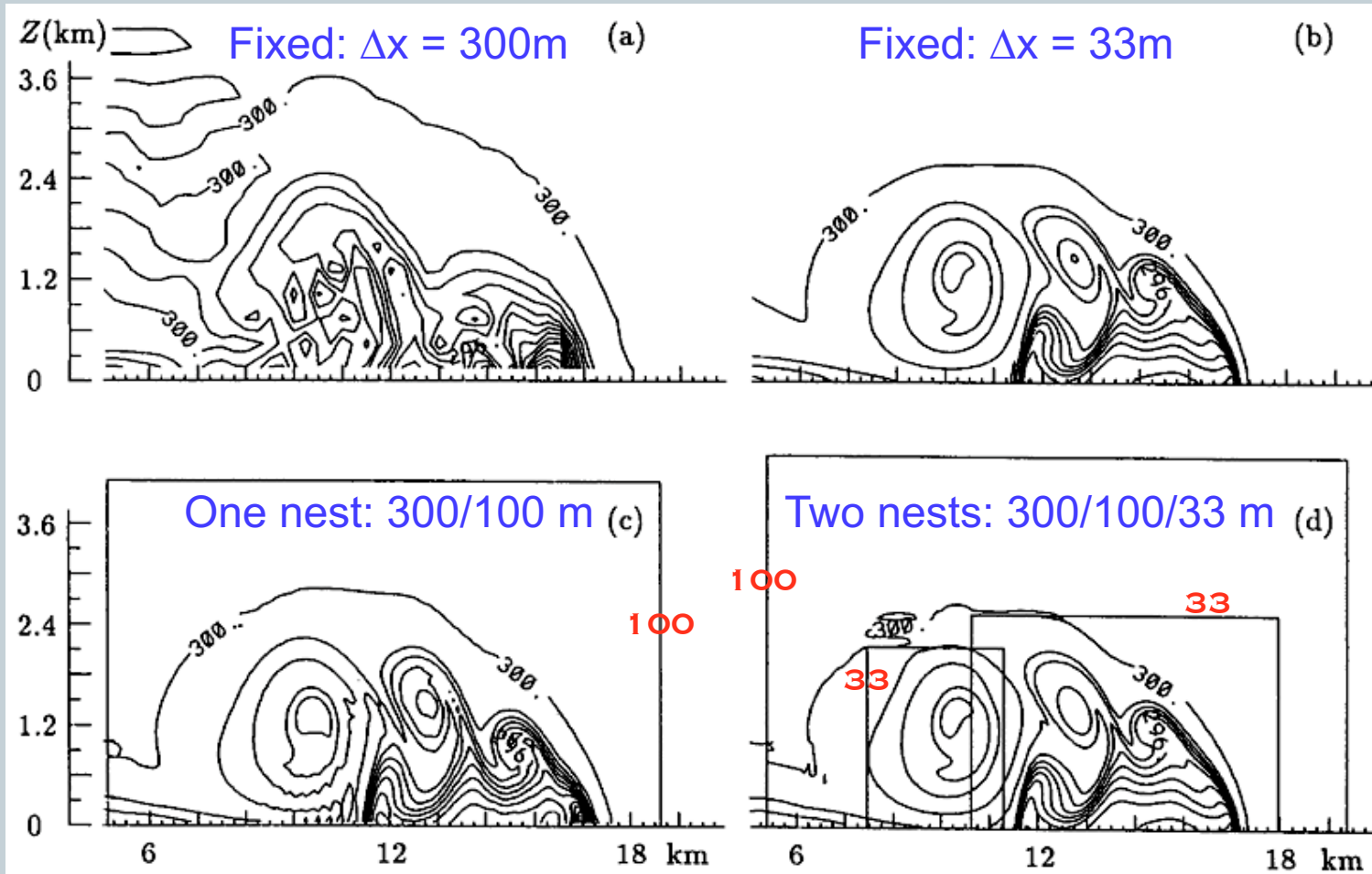
Nesting strategy

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- Identification
 - grid points exceeding some threshold, e.g. truncation error
 - Clustering
 - fit to enclose points
 - general AMR allows overlapping grids, arbitrary orientation
 - Nest: Initial conditions
 - Interpolated from coarse grid, or existing nests
 - Nest: Bound. conditions
 - Time dependent
 - ✦ from coarse grid, using current and 'next' step.
 - Spatial dependence
 - ✦ interpolated from coarse grid. in our case, nest BC overlap with coarse points
-
- Feedback: nest to coarse grid
 - Average nest interior to coarse points

Results: 2D outflow problem

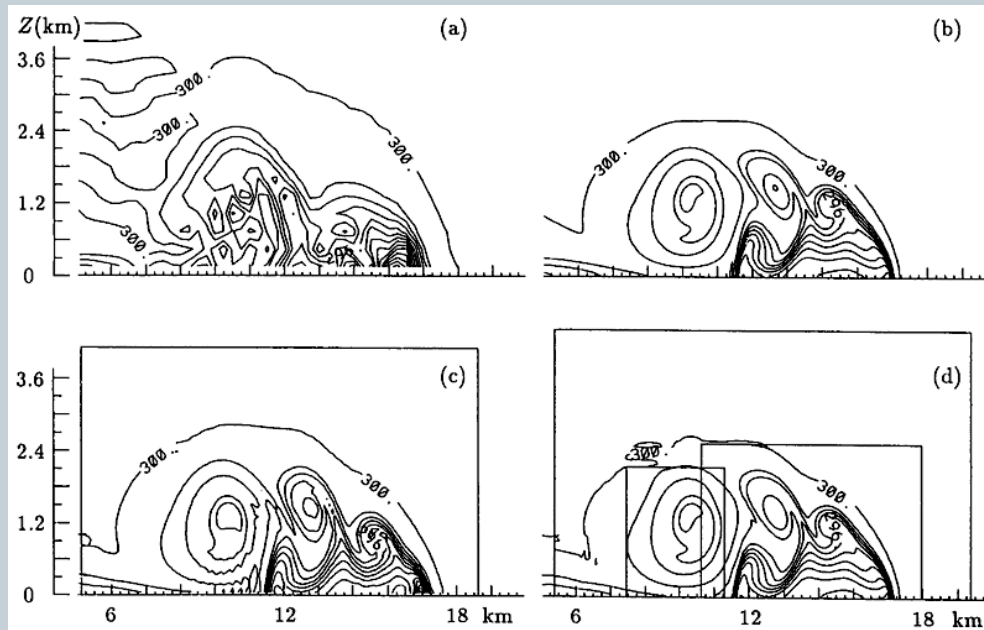
29



How much refinement?

30

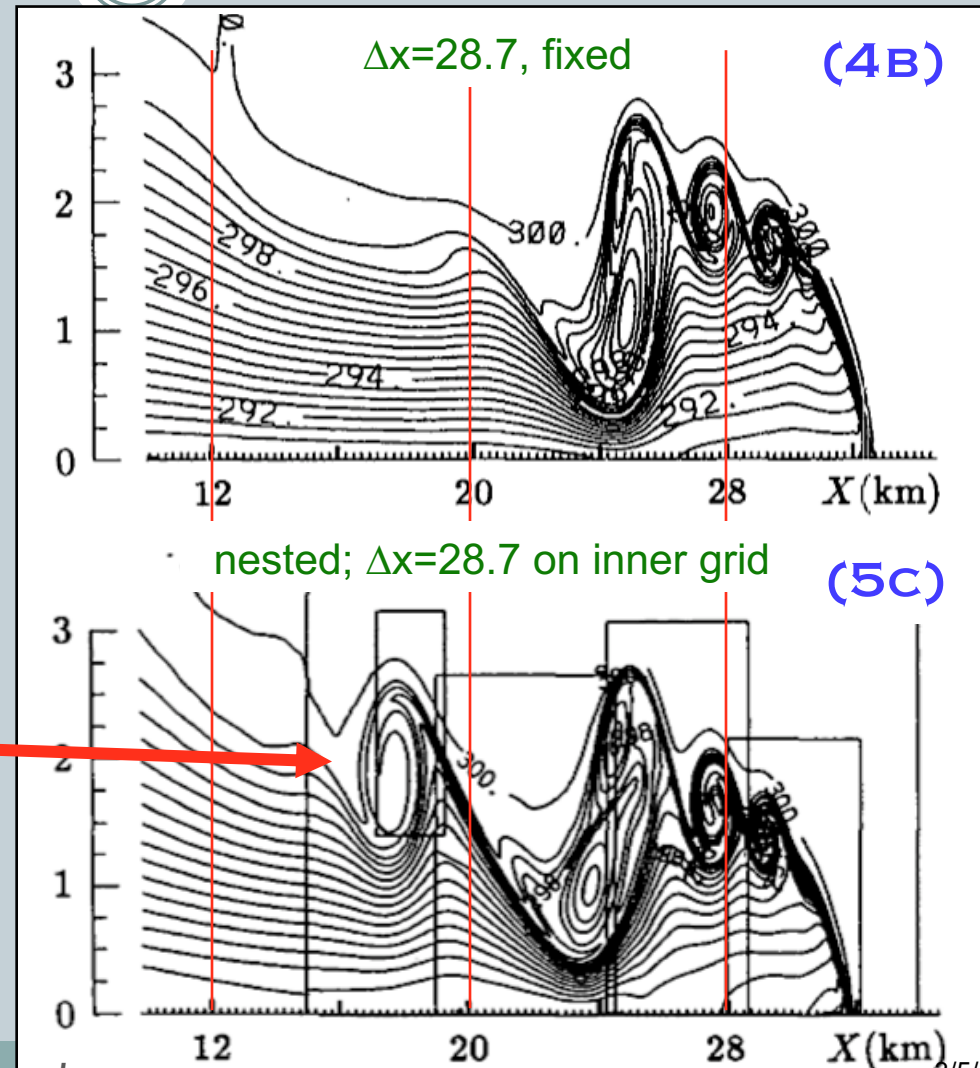
- *Their AMR is a local refinement method!*
 - *efficiency reduced as larger area refined (AMR has a cost)*
 - *break-even: 50-60% of coarse grid refined (= max to refine)*
 - *if you need to refine a bigger area: just refine entire grid*



BC noise, spurious waves

31

- Fixed resolution run shown (top)
- Nested solution shown (bottom)
- Inner nested grid $\Delta x = 28.7\text{m}$
- This is not physical !!!



Parameterization, convergence

32

- **Parameterization of physical processes**
 - this refers to treatment of a sub-grid process using information on larger scales
 - common practice
 - may affect convergence!
- **Truncation error vs. grid size**
 - did not decrease as expected with improved resolution – error sometimes increased!
 - ✦ *as a consequence of grid-scale-dependent parameterizations*
 - smaller $\Delta x \Rightarrow$ smaller-scale features!!