DISCRETE PHYSICAL REALM

ALGEBRAIC FORMULATION OF PHYSICS

A. BÁEZ, F.X. TRIAS AND N. VALLE

Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

Fundació per al Progrés de la Transferència de Calor i Massa

termofluids

FTCM

Fundació per al Progrés de la Transferència de Calor i Massa

CTTC UPC

Centre Tecnològic de Transferència de Calor

UNIVERSITAT POLITÈCNICA DE CATALUNYA

ERRORS, STABILITY AND CODE VERIFICATION

TAMING THE BEAST

"Programming is thinking, not typing."—Casey Patton

ERROR LANDSCAPE

Validation

Solve the right equations

Verification

Solve the equations right

$$\frac{\partial \varphi}{\partial t}+\Gamma\frac{\partial^2 \varphi}{\partial x^2}=f$$

$$\frac{d\varphi_h}{dt}+D\varphi_h=f_h$$

$$Ax=b \Rightarrow x\approx A^{-1}b$$

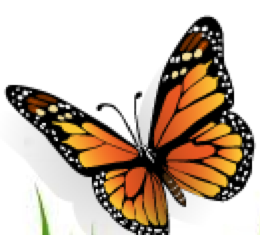
Physical realm → Math model → Discrete eqs. → Numerical solution

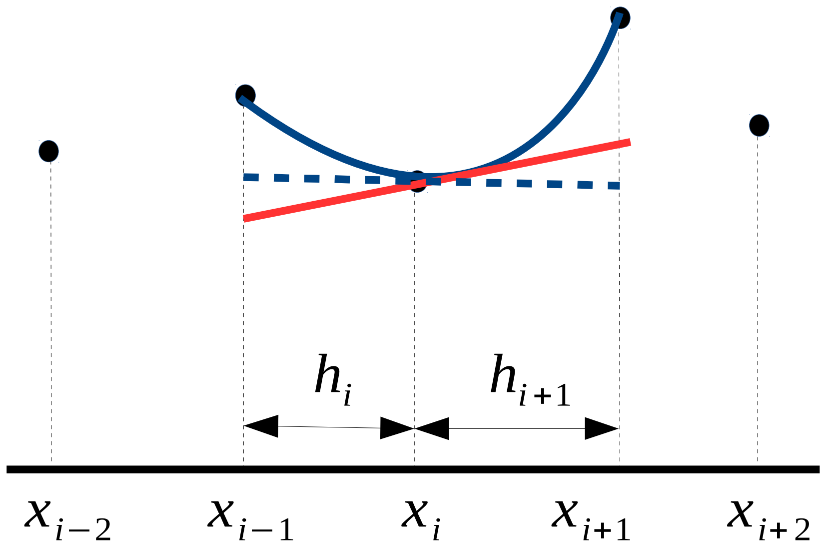
Modelization errors

Discretization errors

- Local truncation error
- Global truncation error
- Dispersion error
- Aliasing error

Solver residual
Round-off errors





$$\left.\frac{\partial \varphi}{\partial x}\right|_{x_i}$$

Taylor series expansion around x_i:

$$\varphi_i = \varphi_i$$

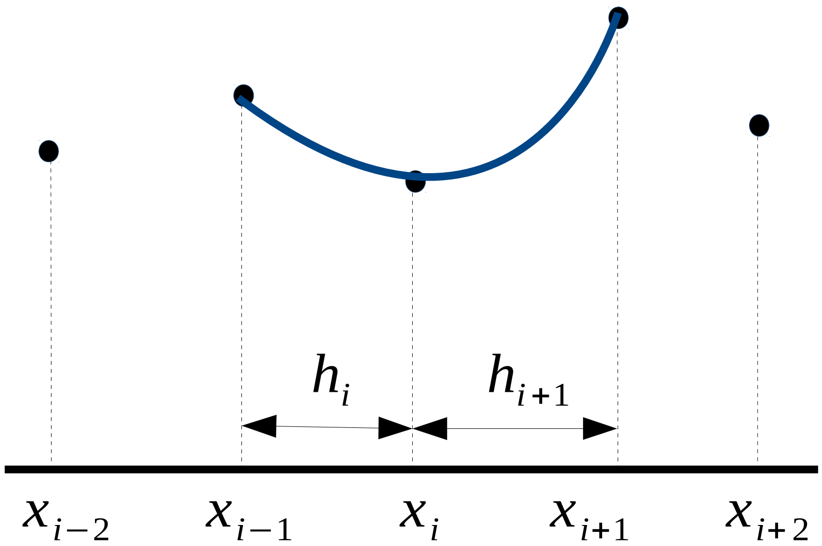
$$\varphi_{i+1} = \varphi_i + h_{i+1} \partial_x \varphi_i + \frac{h_{i+1}^2}{2} \partial_{xx} \varphi_i + \frac{h_{i+1}^3}{3!} \partial_{xxx} \varphi_i + \ldots$$

$$\varphi_{i-1} = \varphi_i - h_i \partial_x \varphi_i + \frac{h_i^2}{2} \partial_{xx} \varphi_i - \frac{h_i^3}{3!} \partial_{xxx} \varphi_i + \ldots$$

$$\left.\frac{\partial \varphi}{\partial x}\right|_{x_i} = \frac{\varphi_{i+1} - \varphi_{i-1}}{h_i + h_{i+1}} + O(h^1)$$

$$\left.\frac{\partial \varphi}{\partial x}\right|_{x_i} = \frac{h_i^2 \varphi_{i+1} + (h_{i+1}^2 - h_i^2) \varphi_i - h_{i+1}^2 \varphi_{i-1}}{h_i h_{i+1} (h_i + h_{i+1})} + O(h^2)$$

CLASSICS: LOCAL TRUNCATION ERROR



$$\left.\frac{\partial^2 \varphi}{\partial x^2}\right|_{x_i}$$

Taylor series expansion around x_i:

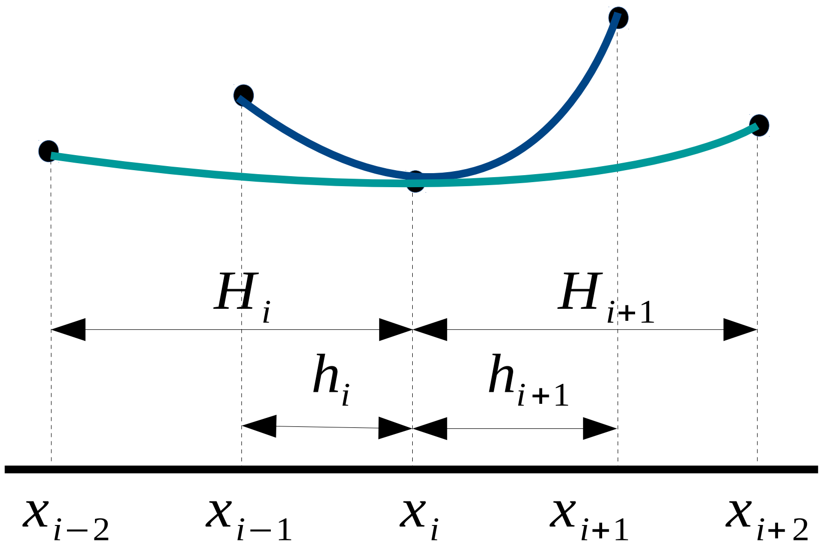
$$\varphi_i \quad = \varphi_i$$

$$\varphi_{i+1} = \varphi_i + h_{i+1}\partial_x \varphi_i + \frac{h_{i+1}^2}{2}\partial_{xx}\varphi_i + \frac{h_{i+1}^3}{3!}\partial_{xxx}\varphi_i + \ldots$$

$$\varphi_{i-1} = \varphi_i - h_i\partial_x \varphi_i + \frac{h_i^2}{2}\partial_{xx}\varphi_i - \frac{h_i^3}{3!}\partial_{xxx}\varphi_i + \ldots$$

$$\begin{pmatrix} 1 & 1 & 1 \\ -h_i & 0 & h_{i+1} \\ h_{i-1}^2/2 & 0 & h_{i+1}^2/2 \end{pmatrix}\begin{pmatrix} c_{i-1} \\ c_i \\ c_{i+1} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \Rightarrow \begin{pmatrix} c_{i-1} \\ c_i \\ c_{i+1} \end{pmatrix} = \frac{1}{h_i h_{i+1}(h_i + h_{i+1})}\begin{pmatrix} h_{i+1} \\ -(h_i + h_{i+1}) \\ h_i \end{pmatrix}$$

$$\left.\frac{\partial^2 \varphi}{\partial x^2}\right|_{x_i} = \frac{h_i \varphi_{i+1} - (h_{i+1} + h_i)\varphi_i + h_{i+1}\varphi_{i-1}}{h_i h_{i+1}(h_i + h_{i+1})} + O(h^2)$$



$$\left.\frac{\partial^2 \varphi}{\partial x^2}\right|_{x_i}$$

...using **Richardson** extrapolation

Taylor series expansion around x_i:

$$\varphi_i = \varphi_i$$

$$\varphi_{i+1} = \varphi_i + h_{i+1}\partial_x \varphi_i + \frac{h_{i+1}^2}{2}\partial_{xx}\varphi_i + \frac{h_{i+1}^3}{3!}\partial_{xxx}\varphi_i + \ldots$$

$$\varphi_{i-1} = \varphi_i - h_i\partial_x \varphi_i + \frac{h_i^2}{2}\partial_{xx}\varphi_i - \frac{h_i^3}{3!}\partial_{xxx}\varphi_i + \ldots$$

$$\left.\frac{\partial^2 \varphi}{\partial x^2}\right|_{x_i} = \frac{\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}}{h^2} + \overbrace{\frac{h^2}{4!}\partial_{xxxx}\varphi_i + O(h^4)}^{\text{Local truncation error}} \qquad \times \; 4/3$$

$$\left.\frac{\partial^2 \varphi}{\partial x^2}\right|_{x_i} = \frac{\varphi_{i+2} - 2\varphi_i + \varphi_{i-2}}{H^2} + \frac{(2h)^2}{4!}\partial_{xxxx}\varphi_i + O(h^4) \qquad \times -1/3$$

$O(h^4)$ *approximation*

CODE VERIFICATION...

...using the Method of Manufactured Solutions (MMS)

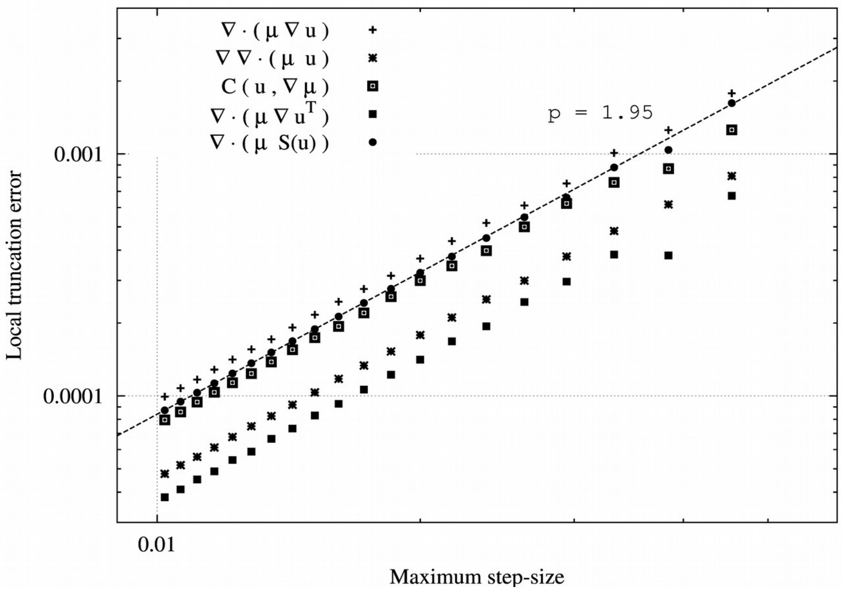
by Eq. (14) was completely straightforward. Then, to measure the order of accuracy of the resulting implementation, a 2D Taylor–Green vortex flow together with the following dynamic viscosity function

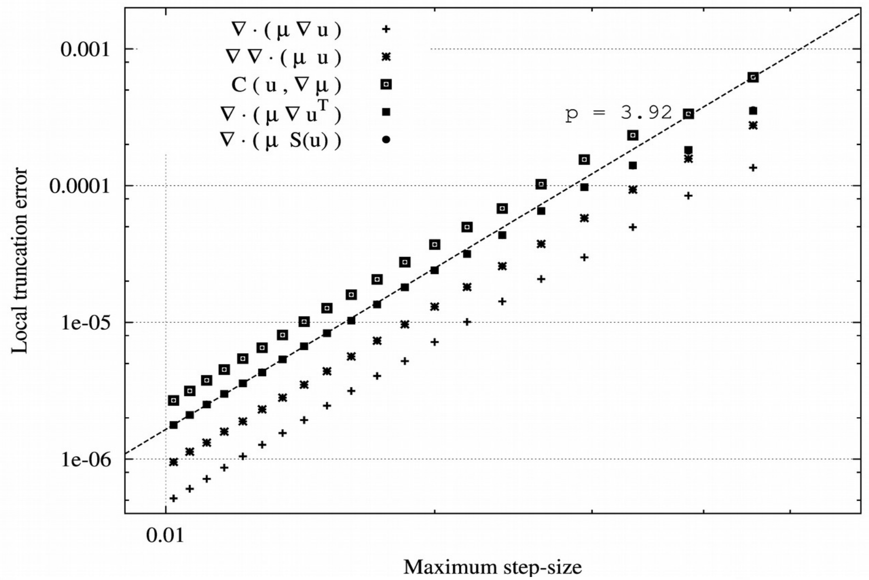
manufactured solution!

$$\boldsymbol{u}_a(\boldsymbol{x}) = 1/A^2\left(-\cos(Ax_1)\sin(Ax_2), \sin(Ax_1)\cos(Ax_2), 0\right), \tag{15a}$$

$$\mu_a(\boldsymbol{x}) = C + \sin(Bx_1)\cos(Bx_2)/B^2, \tag{15b}$$

with $A = 5\pi$, $B = 8\pi$ and $C = 20$, have been used to evaluate the different terms of interest on the bounded square domain





Extracted from F.X. Trias, A. Gorobets and A. Oliva. "A simple approach to discretize the viscous term with spatially varying (eddy-)viscosity", Journal of Computational Physics, 253 (1): 405-417, 2013.

termofluids FTCM
Fundació per al Progrés de la Transferència de Calor i Massa
CTTC UPC
Centre Tecnològic de Transferència de Calor
UNIVERSITAT POLITÈCNICA DE CATALUNYA

What is really important?

Continuous problem: $\nabla^2 \varphi^a = f^a$

Discrete problem: $D\varphi_h = f_h^a$

Local truncation error: $\tau_h = D\varphi_h^a - f_h^a$

Global truncation error: $\varepsilon_h = \varphi_h - \varphi_h^a = D^{-1} f_h^a - \varphi_h^a$

$$\boxed{D\varepsilon_h = \tau_h \quad \Rightarrow \quad \varepsilon_h = D^{-1}\tau_h}$$

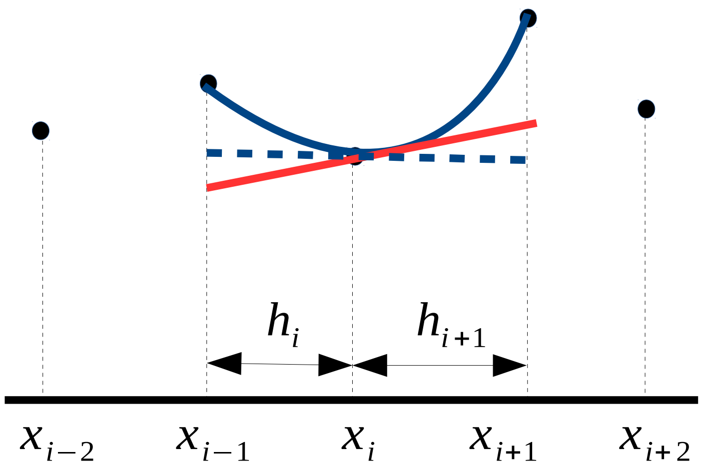
A (nearly) singular discrete operator can destroy the favorable properties of the local truncation error!

termofluids FTCM Fundació per al Progrés de la Transferència de Calor i Massa

CTTC UPC Centre Tecnològic de Transferència de Calor UNIVERSITAT POLITÈCNICA DE CATALUNYA

What is really important?

Of course ε_h



$$\boxed{\Omega^{-1} C \varepsilon_h = \tau_h \;\Rightarrow\; \varepsilon_h = C^{-1} \Omega \tau_h}$$

$$\varepsilon_{i+1} - \varepsilon_{i-1} = 1/2 \left(h_{i+1}^2 - h_i^2\right) \partial_{xx} \varphi_i + O\left(h^3\right)$$

$$\varepsilon_{i+1} - \varepsilon_1 = 1/2 \sum_{k=1}^{i} \left(h_{k+1}^2 - h_k^2\right) \partial_{xx} \varphi_k + O\left(h^2\right)$$

$$= 1/2 \underbrace{\sum_{k=1}^{i-1} h_k^2 \left(\partial_{xx} \varphi_{k-1} - \partial_{xx} \varphi_k\right)}_{O(h^2)} + O\left(h^2\right)$$

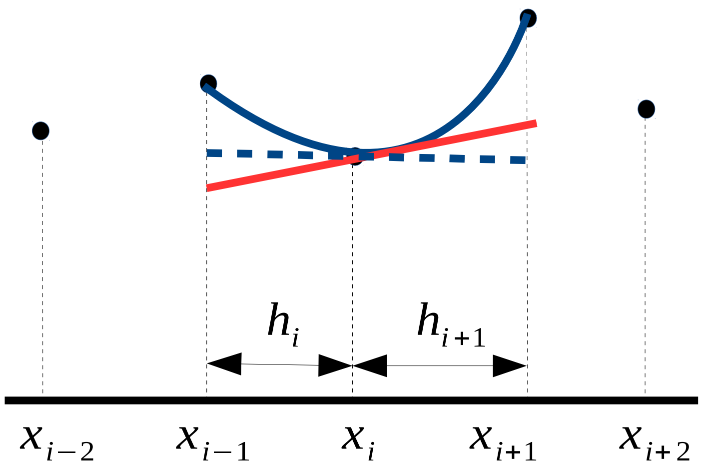
$$\left.\frac{\partial \varphi}{\partial x}\right|_{x_i} = \frac{\varphi_{i+1} - \varphi_{i-1}}{h_i + h_{i+1}} + \overbrace{\frac{h_{i+1} - h_i}{2}}^{1^{st}\ order\ local\ error} \partial_{xx} \varphi_i + O\left(h^2\right)$$

$$\left.\frac{\partial \varphi}{\partial x}\right|_{x_i} = \frac{h_i^2 \varphi_{i+1} + \left(h_{i+1}^2 - h_i^2\right) \varphi_i - h_{i+1}^2 \varphi_{i-1}}{h_i h_{i+1} \left(h_i + h_{i+1}\right)} + O\left(h^2\right)$$

What is really important?

Of course ε_h

$$\boxed{\Omega^{-1} C \varepsilon_h = \tau_h \;\Rightarrow\; \varepsilon_h = C^{-1} \Omega \tau_h}$$



$$\varepsilon_{i+1} - \varepsilon_{i-1} = 1/2\left(h_{i+1}^2 - h_i^2\right)\partial_{xx}\varphi_i + O\left(h^3\right)$$

$$\varepsilon_{i+1} - \varepsilon_1 = 1/2\sum_{k=1}^{i}\left(h_{k+1}^2 - h_k^2\right)\partial_{xx}\varphi_k + O\left(h^2\right)$$

$$= 1/2\underbrace{\sum_{k=1}^{i-1} h_k^2\left(\partial_{xx}\varphi_{k-1} - \partial_{xx}\varphi_k\right)}_{O(h^2)} + O\left(h^2\right)$$

$$\left.\frac{\partial \varphi}{\partial x}\right|_{x_i} = \frac{\varphi_{i+1} - \varphi_{i-1}}{h_i + h_{i+1}} + \overbrace{\frac{h_{i+1} - h_i}{2}}^{1^{st}\ \text{order local error}}\partial_{xx}\varphi_i + O\left(h^2\right)$$

$$\left.\frac{\partial \varphi}{\partial x}\right|_{x_i} = \frac{h_i^2\varphi_{i+1} + \left(h_{i+1}^2 - h_i^2\right)\varphi_i - h_{i+1}^2\varphi_{i-1}}{h_i h_{i+1}\left(h_i + h_{i+1}\right)} + O\left(h^2\right)$$

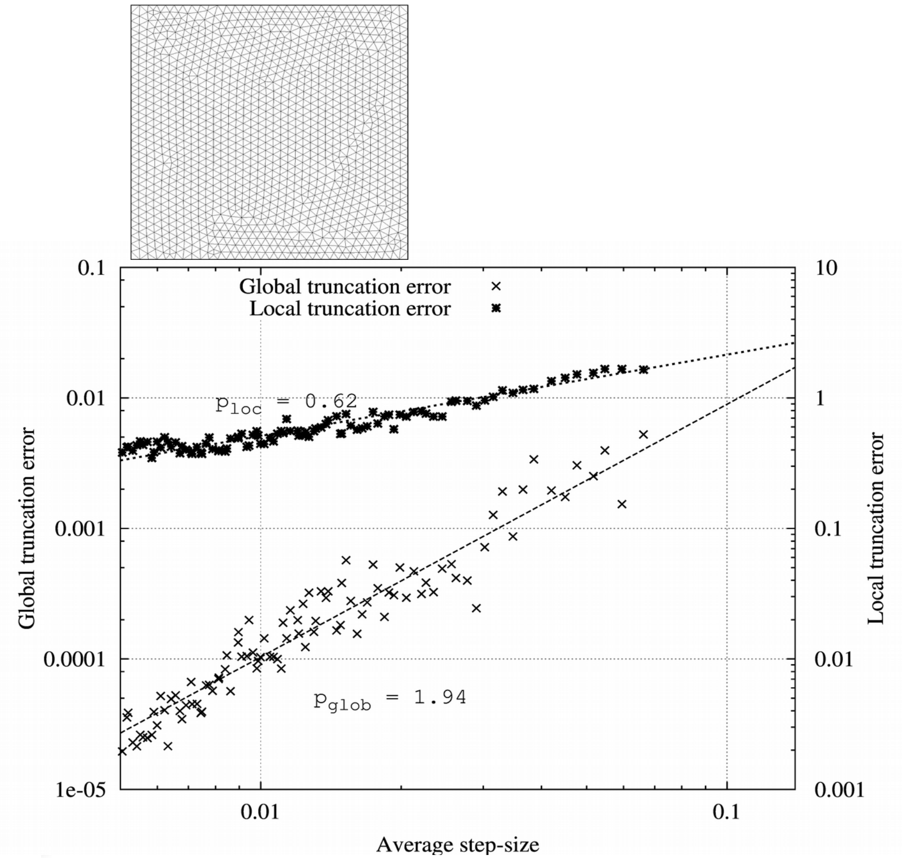
LOCAL VS GLOBAL TRUNCATION ERROR

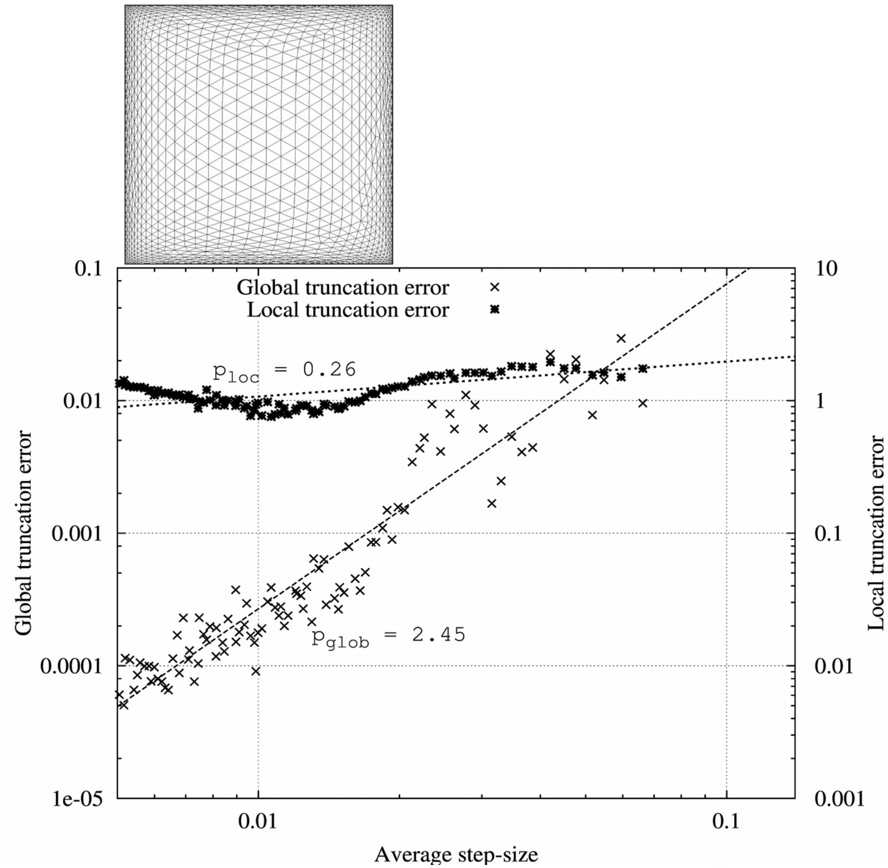
A complete analytical approach for the general case is beyond the scope of this paper. Instead, the following problem

manufactured solution!

$$\Delta\varphi = f \quad \text{on } \Omega = (0,1)\times(0,1) \quad \text{and} \quad \varphi|_{\partial\Omega} = 0, \tag{58}$$

with $f(x_1, x_2) = \Delta(A^{-2}\sin(Ax_1)\sin(Ax_2))$ and $A = 25\pi$ has been numerically solved on 150 different meshes using the discrete approximation of the Laplacian operator defined in Eq. (46). The ANSYS ICEM CFD package has been used to ran-





Extracted from F.X. Trias, O. Lehmkuhl, A. Oliva, C.D. Pérez-Segarra and R.W.C.P. Verstappen. "Symmetry-preserving discretization of Navier-Stokes equations on collocated unstructured grids", Journal of Computational Physics, 258 (1): 246-267, 2014.

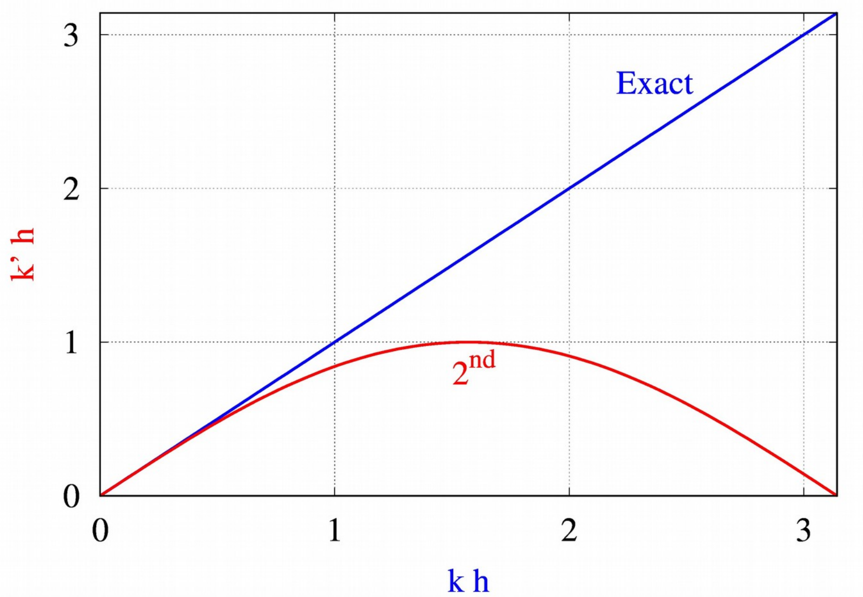
DISPERSION ERROR

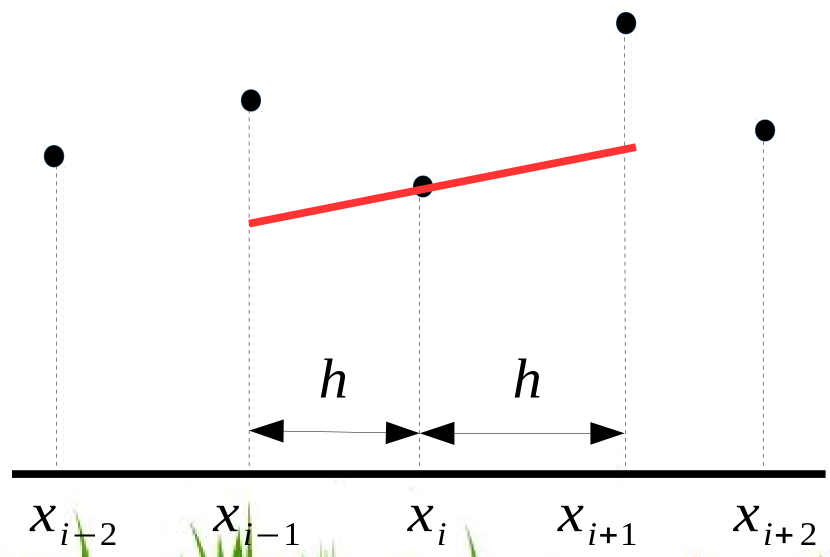
Let us consider a single wave: $\varphi(x)=e^{ikx} \Rightarrow \partial_x \varphi(x) = i k \varphi(x)$

modified wavenumber

Second-order central difference:

$$\left.\frac{\partial\varphi}{\partial x}\right|_{x_i} = \frac{\varphi_{i+1}-\varphi_{i-1}}{2h} = \frac{e^{ik(x_i+h)}-e^{ik(x_i-h)}}{2h} = \frac{e^{ikh}-e^{-ikh}}{2h}\, e^{ikx_i} = i\, \overbrace{\frac{\sin(hk)}{h}}^{k'}\, \varphi_i$$





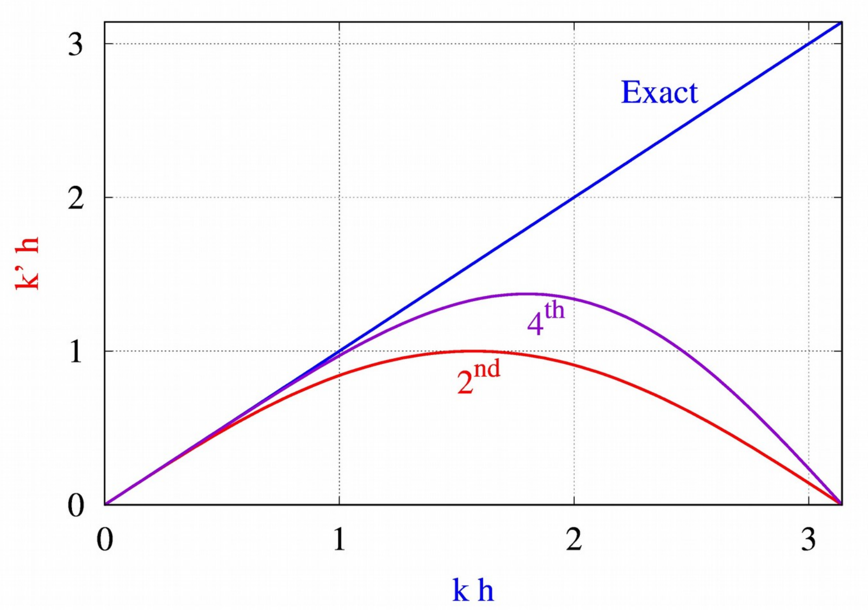
DISPERSION ERROR

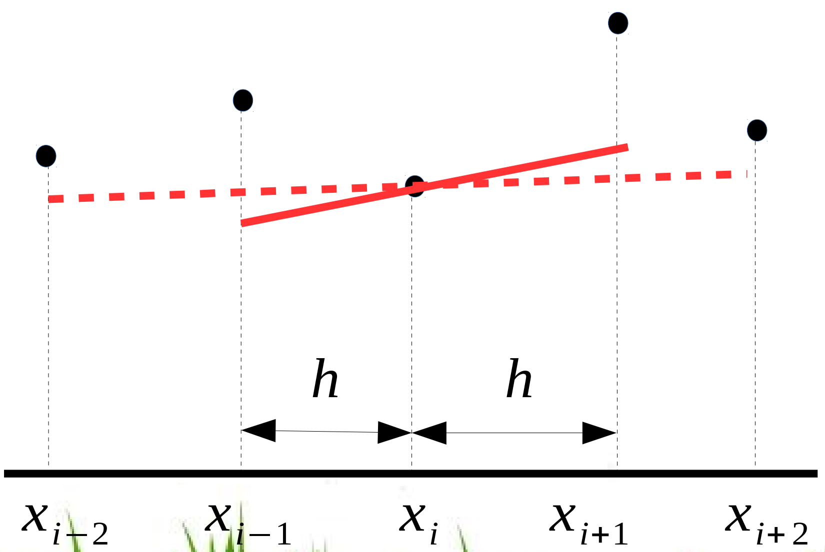
Fourth-order central difference:

$$\left.\frac{\partial \varphi}{\partial x}\right|_{x_i} = \frac{-\varphi_{i+2} + 8\varphi_{i+1} - 8\varphi_{i-1} + \varphi_{i+2}}{12h} = \left(\frac{e^{ikh} - e^{-ikh}}{3h/2} - \frac{e^{ik2h} - e^{-ik2h}}{12h} \right) \varphi_i$$

$$= i \underbrace{\left(\frac{4\sin(hk)}{3h} - \frac{\sin(2hk)}{6h} \right)}_{k'} \varphi_i$$

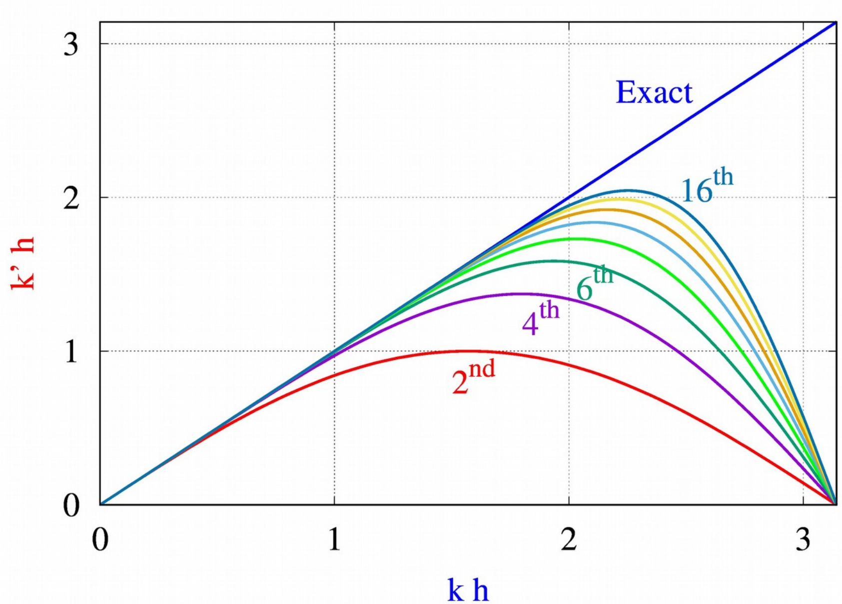
modified wavenumber

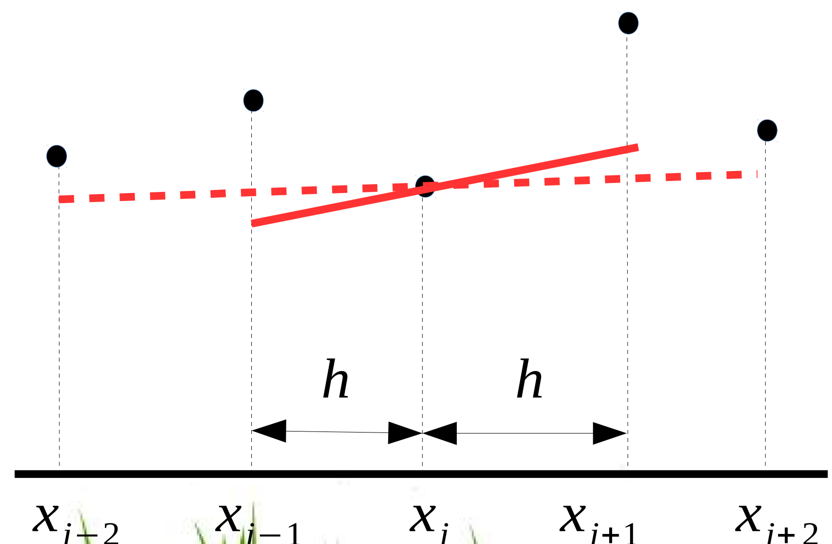




Increasing order of accuracy helps…

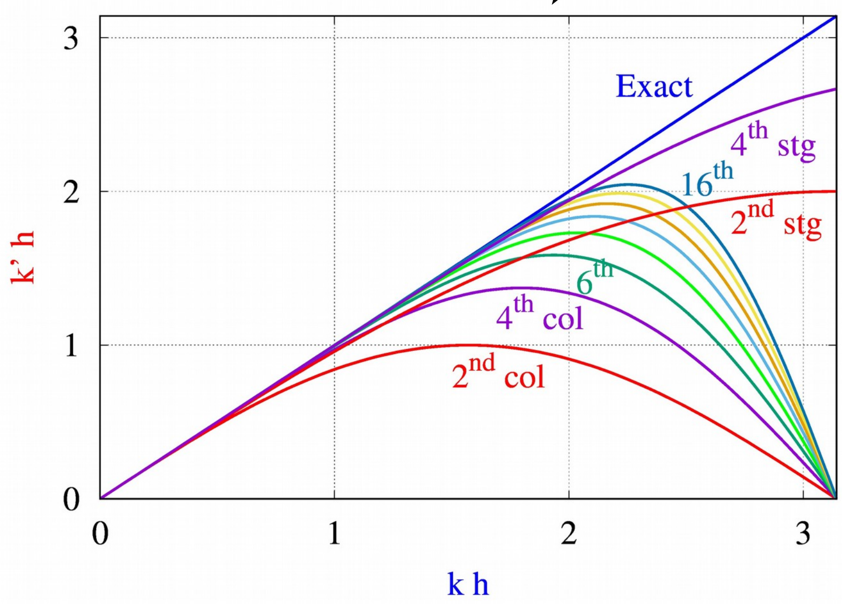
… but it is so expensive!

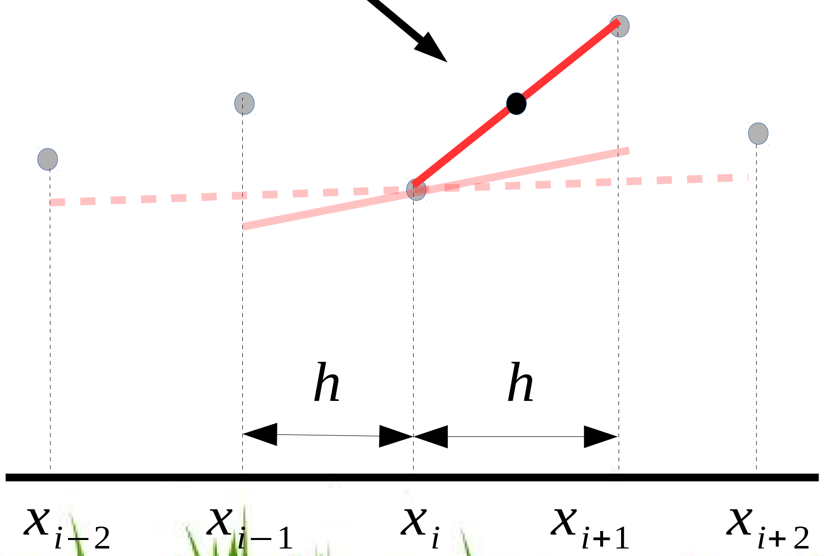




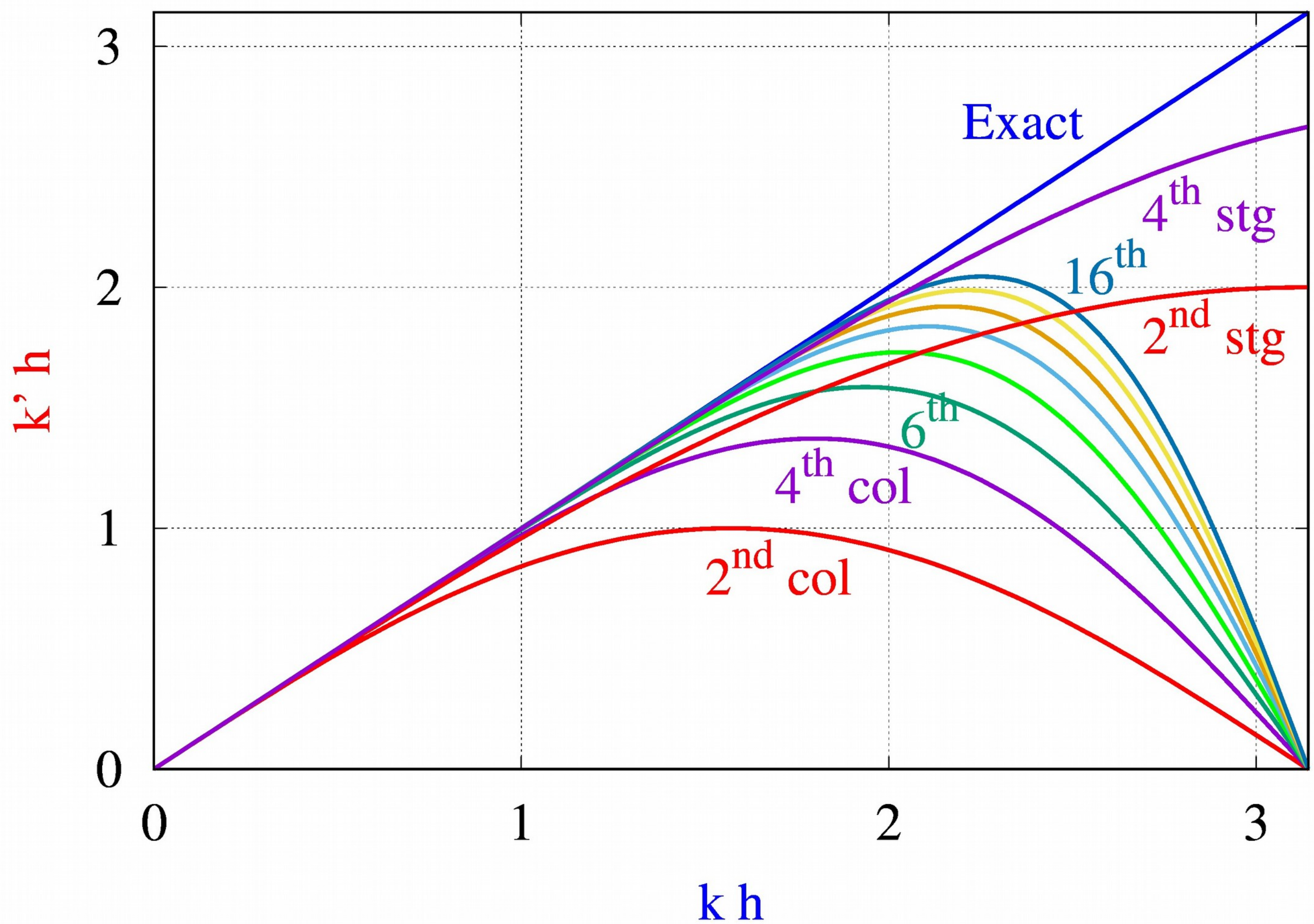
Here you can see (again) the benefits of using a **staggered** arrangement!

It is equivalent to increase mesh resolution by a factor of 2!





But why dispersion errors are important?



DISPERSION ERROR

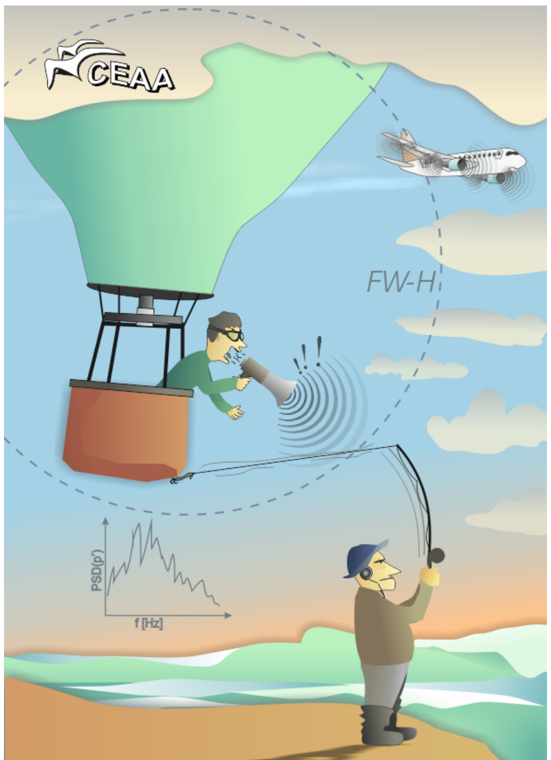
Let us consider a single wave traveling at speed U :

$$\varphi(x,t)=e^{ik(x-Ut)} \Rightarrow \partial_t \varphi = U\,\partial_x \varphi = i\,k\,U\,\varphi$$

$$\Rightarrow \partial_t \varphi = U\,\hat{\partial}_x \varphi = i\,k'U\,\varphi \quad \text{Dispersion error}$$

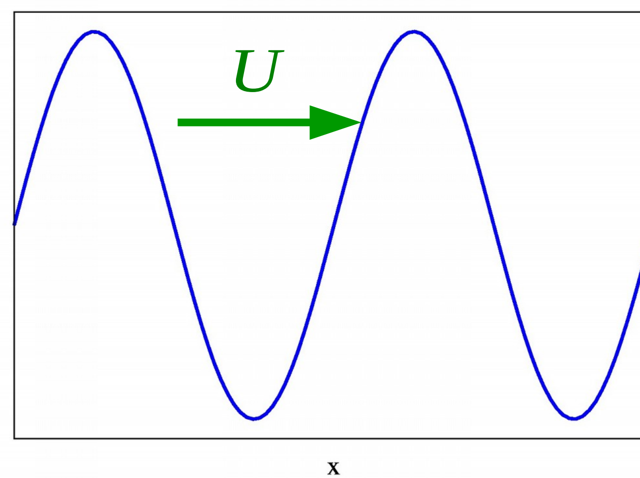
$$\Rightarrow \partial_t \varphi = U'\partial_x \varphi = i\,\underbrace{k\;U'}\,\varphi \quad \text{Doppler effect}$$

Actual measured wavenumber



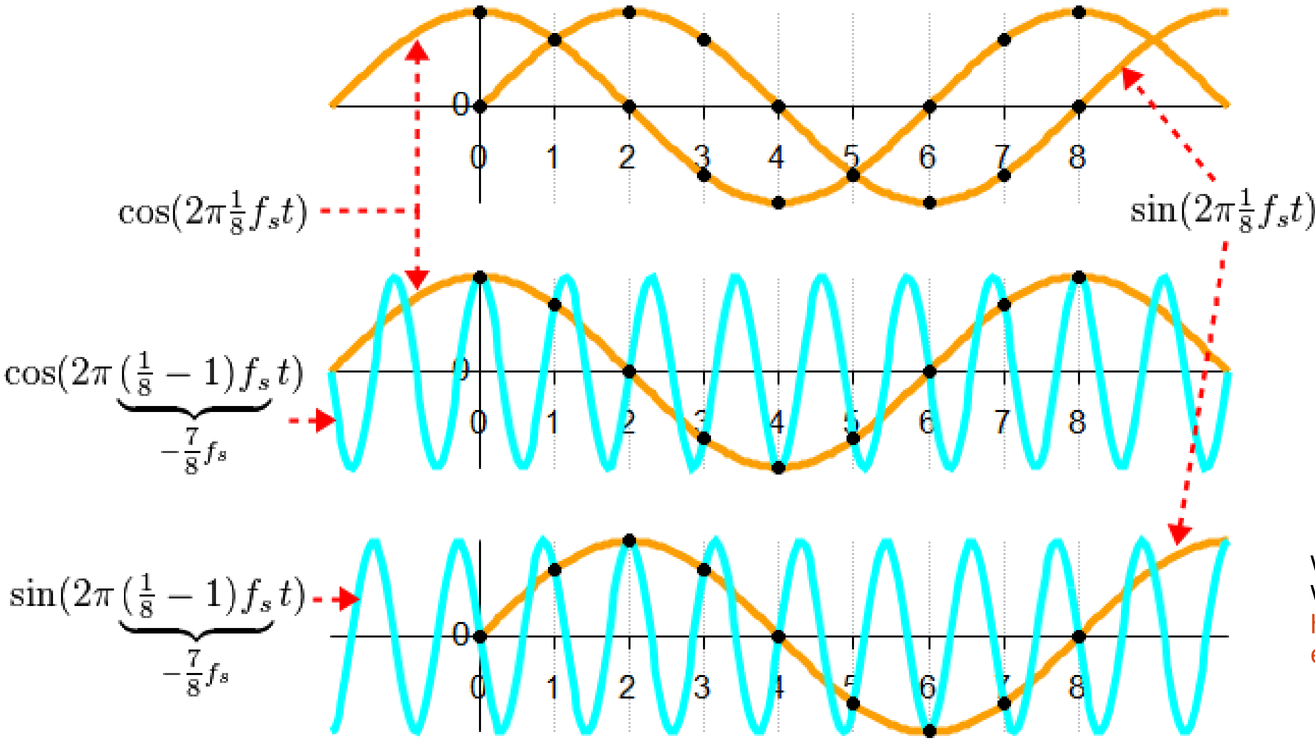
Cover of the Fourth International Workshop Computational Experiment in AeroAcoustics, Svetlogorsk, Russia, September 2016.

By Dr.Sci.Andrey Gorobets



ALIASING ERROR

It is simply due to under-sampling



Wikipedia contributors, "Aliasing," Wikipedia, The Free Encyclopedia, https://en.wikipedia.org/w/index.php?title=Aliasing&oldid=749178544 (accessed February 24, 2017).

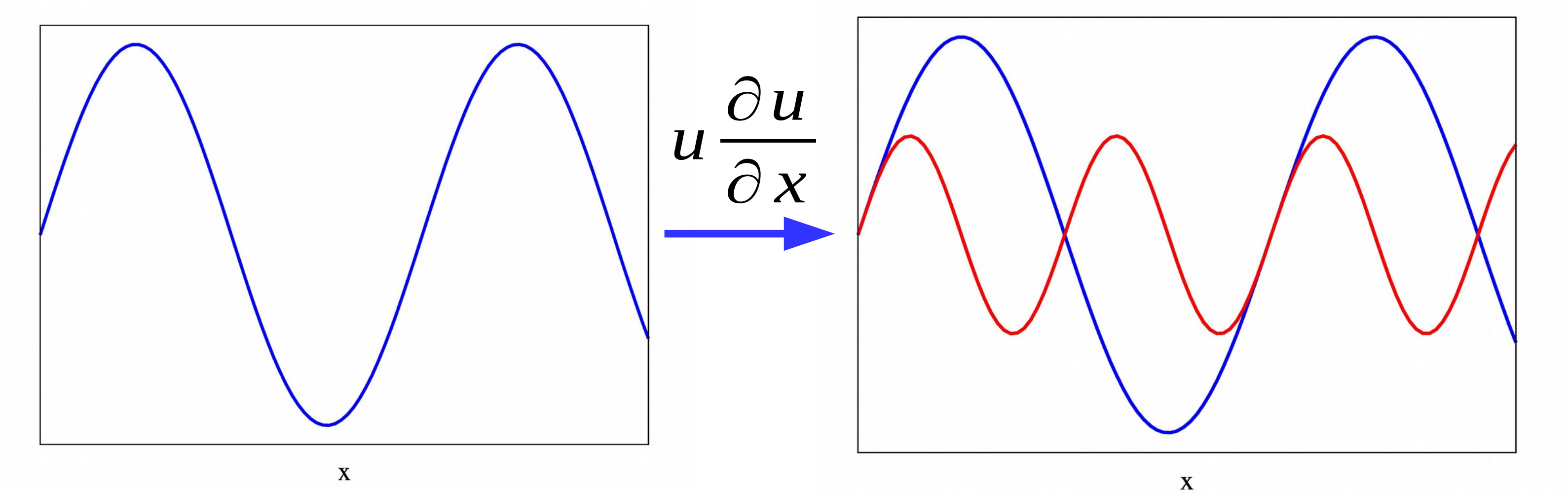
But who can create over-sampled signals?

ALIASING ERROR

Of course, our **non-linear** friend!

Let us consider a one single 1D wave, $u(x)=\sin(\boldsymbol{k}\,x)$

$$u\frac{\partial u}{\partial x}=k\sin(k\,x)\cos(k\,x)=\frac{k}{2}\sin(\mathbf{2}\boldsymbol{k}\,x)$$



$$\frac{\partial\vec{u}}{\partial t}+\underbrace{(\vec{u}\cdot\nabla)\vec{u}}_{\text{nonlinear guy in NS}}=\nu\nabla^2\vec{u}-\nabla p\,;\qquad \nabla\cdot\vec{u}=0$$

REMAINDERS!!!

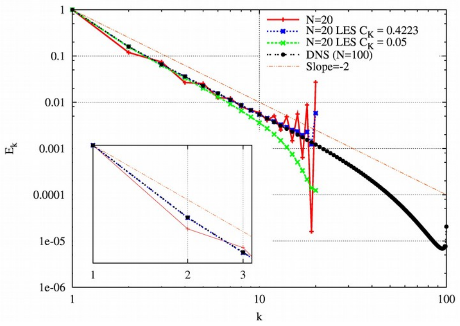
Double-angle formula: $\sin(2x)=2\sin(x)\cos(x)$

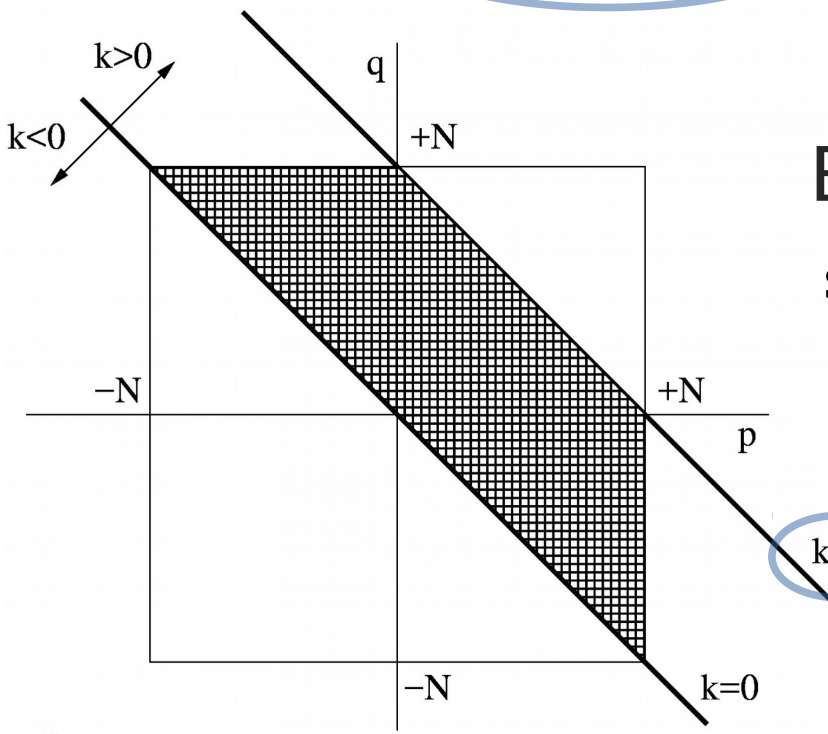
termofluids FTCM Fundació per al Progrés de la Transferència de Calor i Massa

CTTC UPC Centre Tecnològic de Transferència de Calor UNIVERSITAT POLITÈCNICA DE CATALUNYA

Of course, our **non-linear** friend!

$$\partial_t \hat{u}_k + \sum_{k=p+q}^{N} \hat{u}_p \, i q \, \hat{u}_q = -\nu k^2 \hat{u}_k + \hat{f}_k$$





Easy to remember:

$$\sin((2N-k)x_n) = \sin(2\pi n - k x_n) = -\sin(k x_n)$$

Nyquist frequency

$$N = \frac{\pi}{h} \quad \text{and} \quad x_n = x_0 + n h$$

ODDS AND EVENS

$$\left.\frac{\partial \varphi}{\partial x}\right|_{x_i} = \frac{\varphi_{i+1} - \varphi_{i-1}}{2h} + \overbrace{\frac{h^2}{3!}\partial_{xxx}\varphi_i + O(h^4)}^{\textit{Odd local truncation error}}$$

$$\left.\frac{\partial^2 \varphi}{\partial x^2}\right|_{x_i} = \frac{\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}}{h^2} + \overbrace{\frac{h^2}{4!}\partial_{xxxx}\varphi_i + O(h^4)}^{\textit{Even local truncation error}}$$

Let us consider a single wave: $\varphi(x) = e^{i\boldsymbol{k}x}$

$$\partial_x \varphi(x) = i\boldsymbol{k}\varphi(x)$$

$$\partial_{xx} \varphi(x) = -\boldsymbol{k}^2\varphi(x)$$

$$\partial_{xxx} \varphi(x) = -i\boldsymbol{k}^3\varphi(x)$$

$$\partial_{xxxx} \varphi(x) = \boldsymbol{k}^4\varphi(x)$$

...

Transport
Dispersion errors
Wiggles

Diffusion-like
Dissipation errors
Hyper-viscosity...

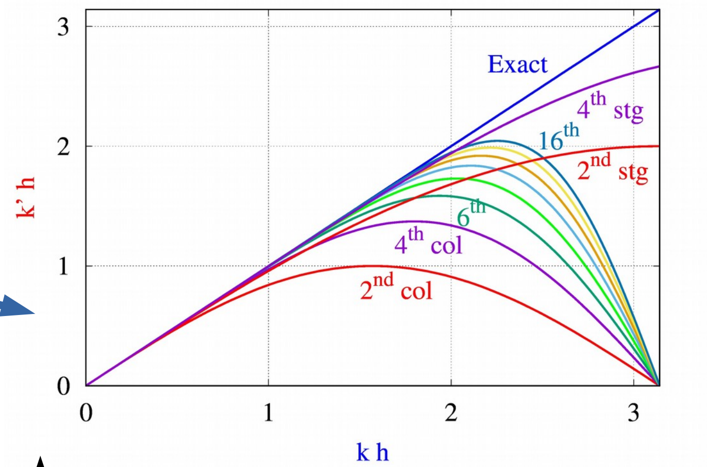
Wikipedia contributors, "Odds and evens," Wikipedia, The Free Encyclopedia, https://en.wikipedia.org/w/index.php?title=Odds_and_evens&oldid=754671496 (accessed February 27, 2017).

ODDS AND EVENS

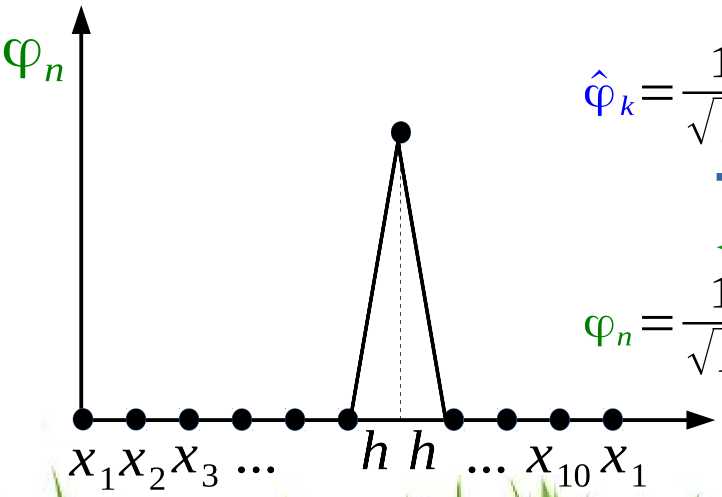
EVEN derivatives are amenable for numerical methods…

but they suffer with ODD derivatives

We have seen that they introduce dispersion errors

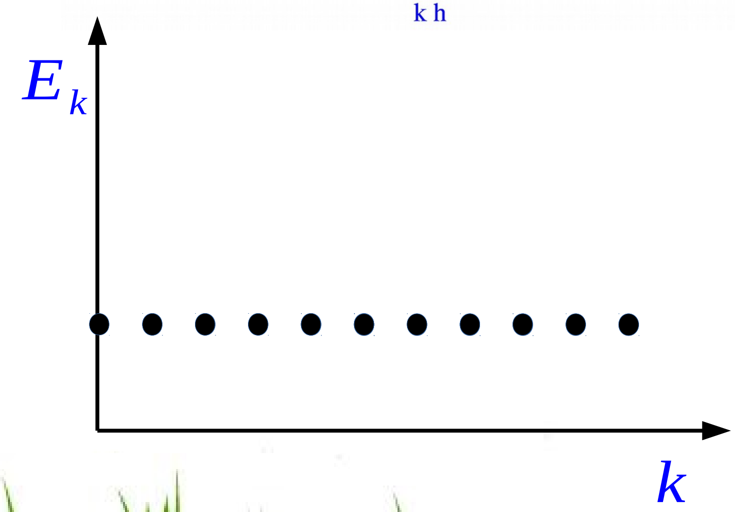


But peaks are even worse… why?



$$\hat{\varphi}_k = \frac{1}{\sqrt{N}} \sum_{n=0}^{n=N} \varphi_n e^{-i\boldsymbol{k} x_n}$$

$$\varphi_n = \frac{1}{\sqrt{N}} \sum_{\boldsymbol{k}=-N}^{\boldsymbol{k}=+N} \hat{\varphi}_k e^{i\boldsymbol{k} x_n}$$

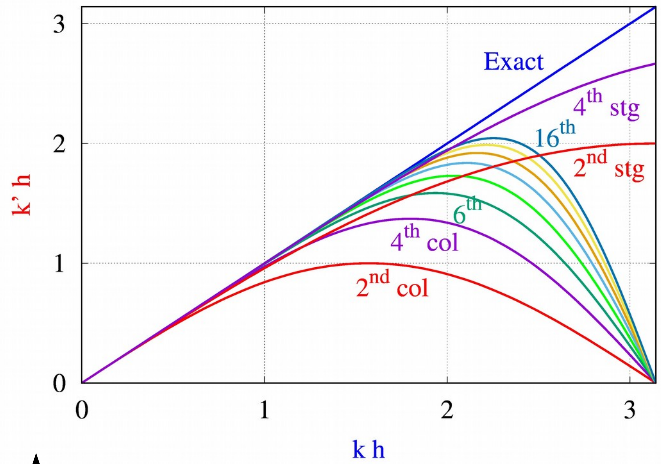


$$E_k \equiv \hat{\varphi}_k \overline{\hat{\varphi}_k}$$

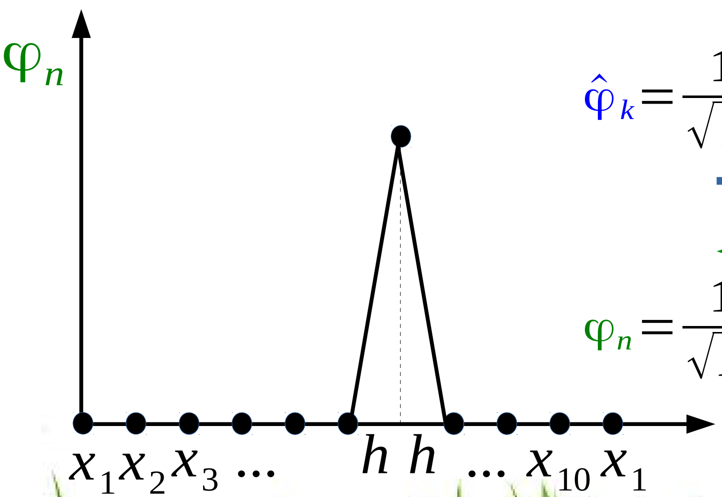
$$\sigma_{\varphi} = \|\varphi - \langle \varphi \rangle\|^2 \geq O(h^2) \qquad \sigma_{\hat{\varphi}} = \|\hat{\varphi} - \langle \hat{\varphi} \rangle\|^2 \geq O(h^2)$$

Heisenberg-Weyl inequality:

$$\|\varphi - \langle \varphi \rangle\|^2 \, \|\hat{\varphi} - \langle \hat{\varphi} \rangle\|^2 \geq \frac{1}{4L}$$

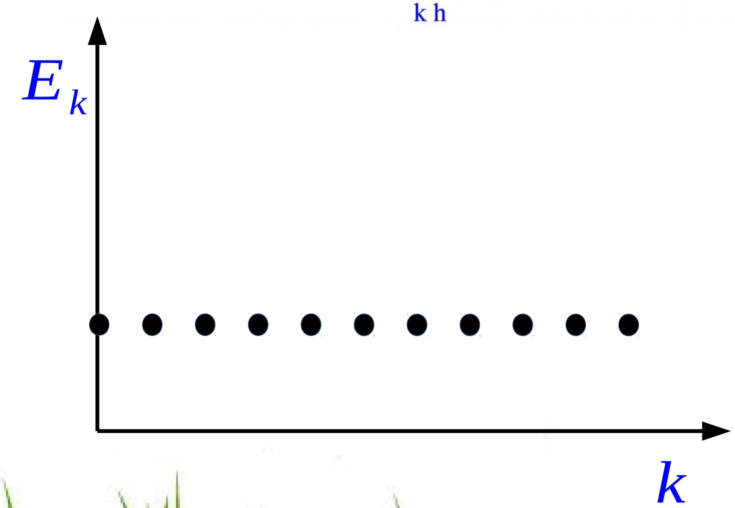


This is an intrinsic problem:
it cannot be solved



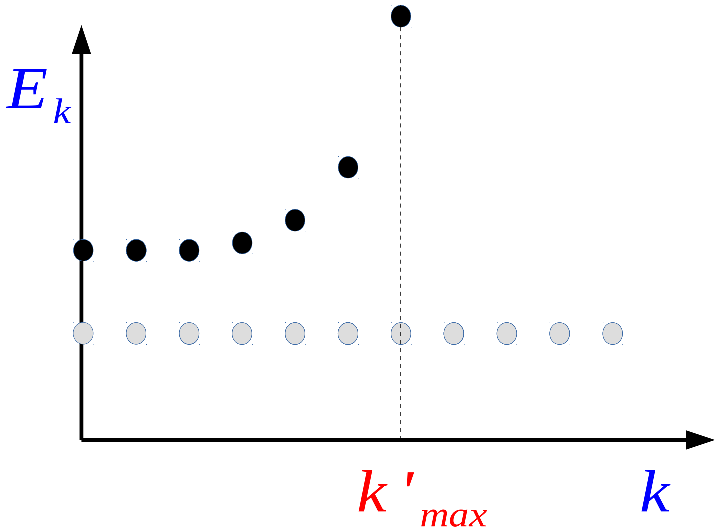
$$\hat{\varphi}_k = \frac{1}{\sqrt{N}} \sum_{n=0}^{n=N} \varphi_n e^{-i\mathbf{k} x_n}$$

$$\varphi_n = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}=-N}^{\mathbf{k}=+N} \hat{\varphi}_k e^{i\mathbf{k} x_n}$$

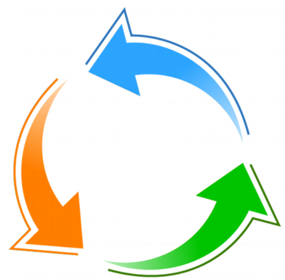


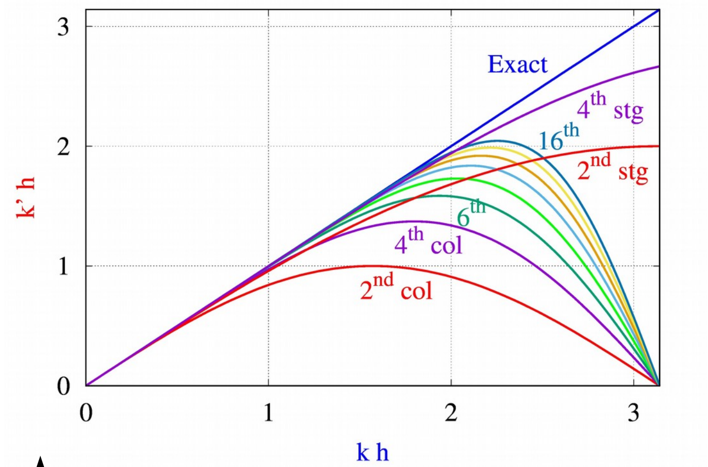
$$E_k \equiv \hat{\varphi}_k \overline{\hat{\varphi}_k}$$

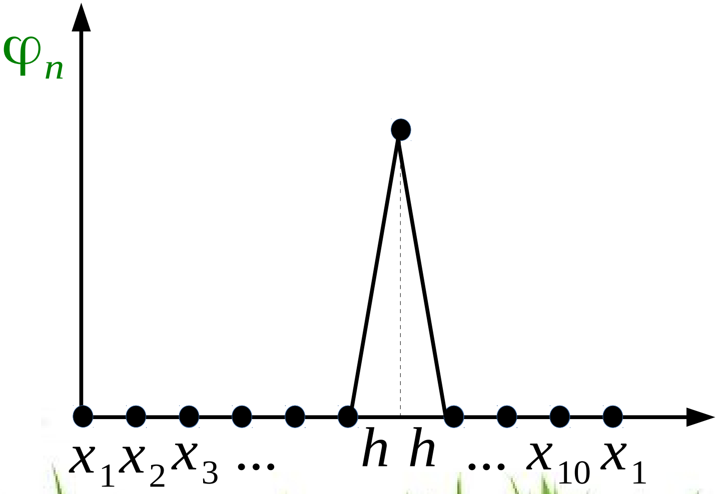
ODDS AND EVENS

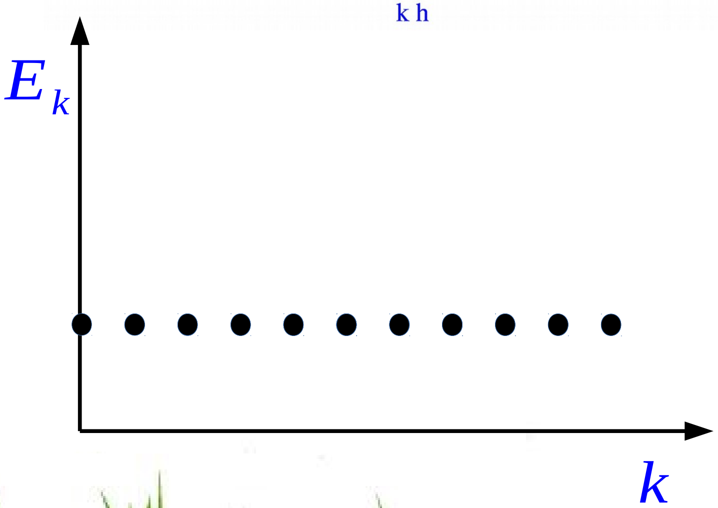


Wiggles ++

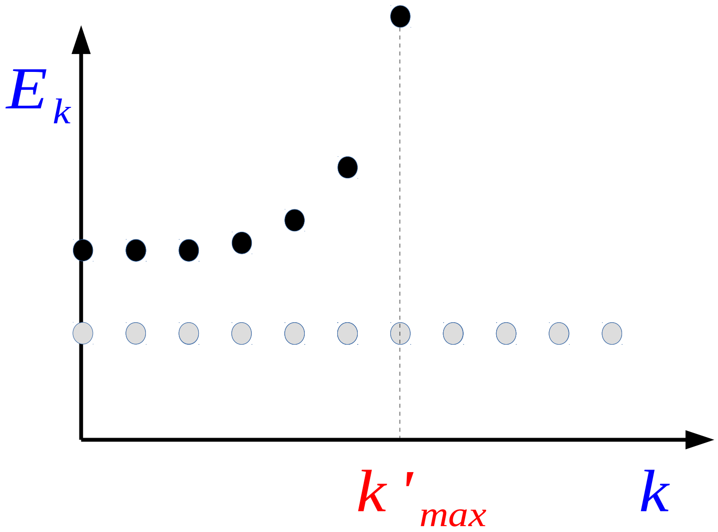




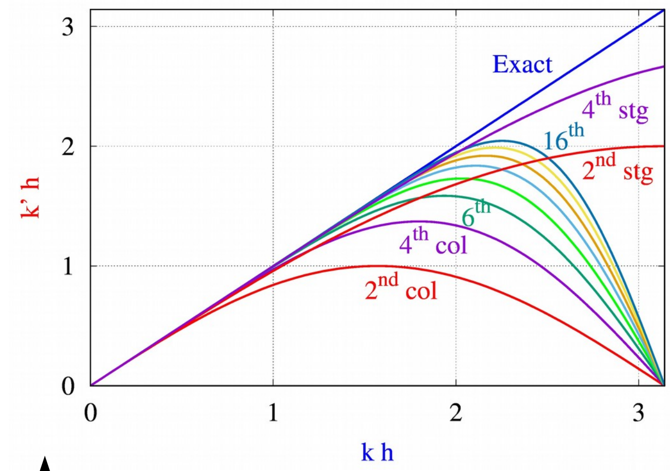




ODDS AND EVENS



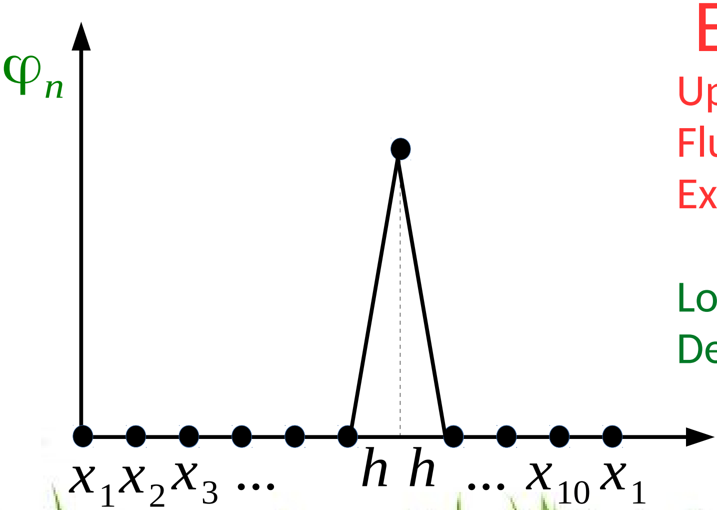
Wiggles --

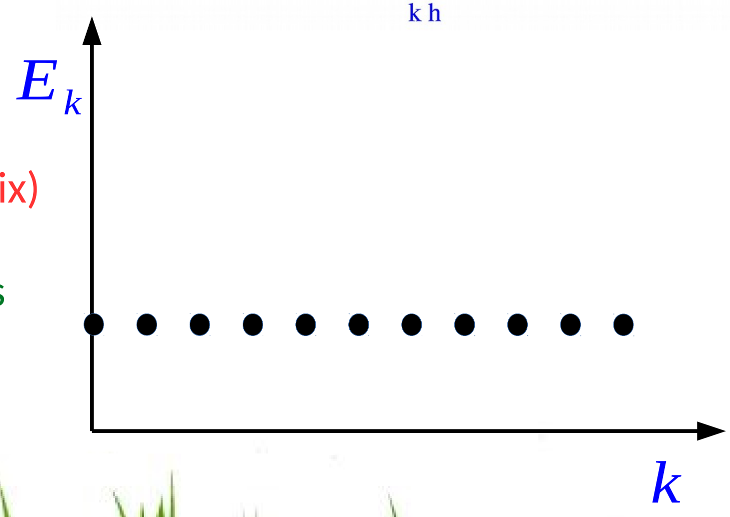


Evens vs odds

Upwind-like schemes
Flux limiters
Explicit filtering (ask Aleix)

Low-dispersion schemes
Dealising techniques



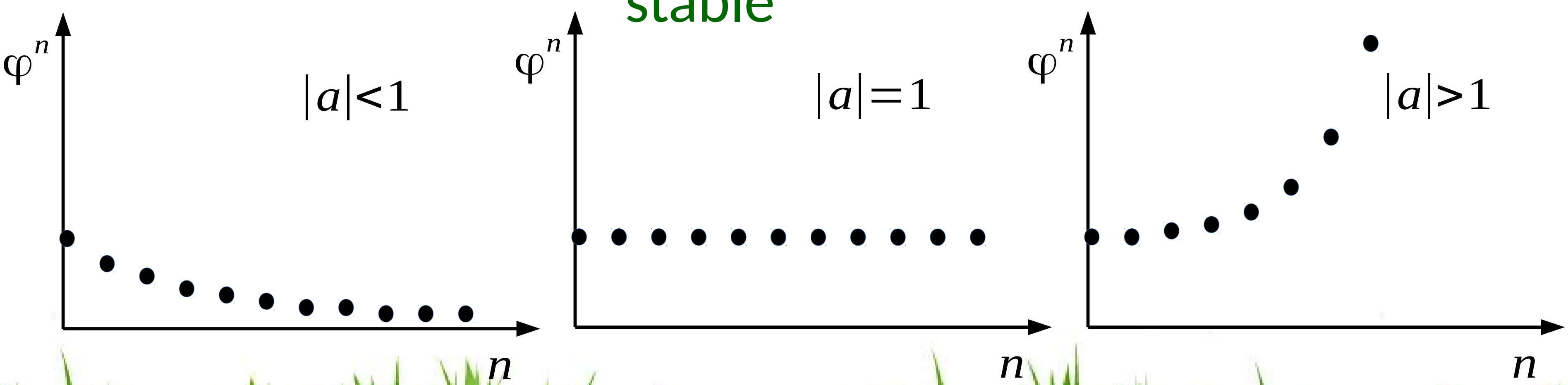


A simulation might blow up, but **you MUST know why**

Preview of ideas:

$$\varphi^{n+1} = a\,\varphi^{n} \quad \text{is stable if } |a| \leq 1$$

Stable | Marginally stable | Unstable



So, at the end, we just need to know the **spectral radius** of our **transfer function**

$$\varphi^{n+1} = f(\varphi^n) \quad \text{is stable if } |f| = |\lambda_{max}| \leq 1$$

$$\varphi^{n+1} = a\varphi^n \quad \text{is stable if } |a| \leq 1$$

$$\varphi_h^{n+1} = \boldsymbol{A}\varphi_h^n \quad \text{is stable if } |\boldsymbol{A}| = |\lambda_{max}| \leq 1$$

Hence, it is basically an **eigenvalue problem** (ask Nico)

Nothing more, nothing else!

STABILITY

Most typical example is **explicit time-integration**

$$\boxed{\varphi_t = \lambda \varphi}$$

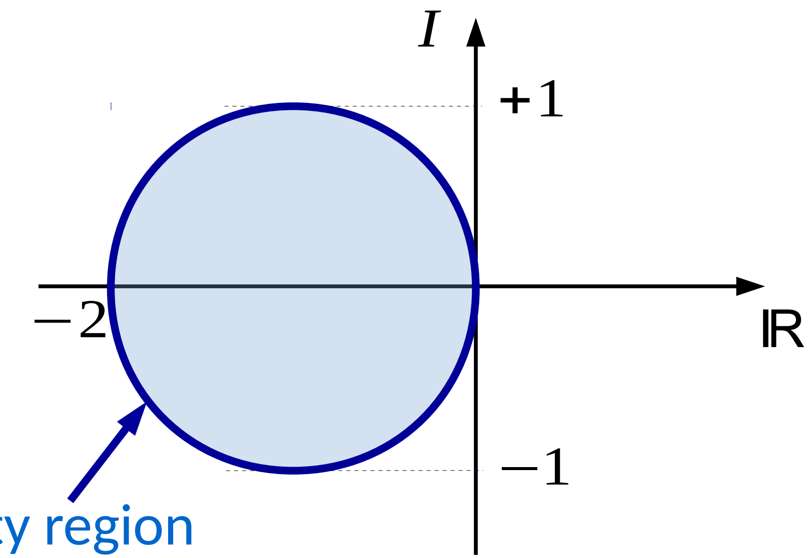
First-order Euler scheme

$$\frac{\varphi^{n+1} - \varphi^{n}}{\Delta t} = \lambda \varphi^{n}$$

transfer function

$$\varphi^{n+1} = (1 + \lambda \Delta t)\varphi^{n}$$

$$\tilde{\lambda} \equiv \lambda \Delta t$$



$$|1 + \tilde{\lambda}| \leq 1$$

Stability region

Most typical example is **explicit time-integration**

$$\boxed{\varphi_t = \lambda \varphi}$$

2nd-order Adams-Bashforth

$$\frac{\varphi^{n+1} - \varphi^{n}}{\Delta t} = \lambda \left(\frac{3}{2} \varphi^{n} - \frac{1}{2} \varphi^{n-1} \right)$$

$$\begin{pmatrix} \varphi^{n+1} \\ \varphi^{n} \end{pmatrix} = \begin{pmatrix} 1 + 3\tilde{\lambda}/2 & -\tilde{\lambda}/2 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \varphi^{n} \\ \varphi^{n-1} \end{pmatrix} \qquad \tilde{\lambda} \equiv \lambda \Delta t$$

transfer function

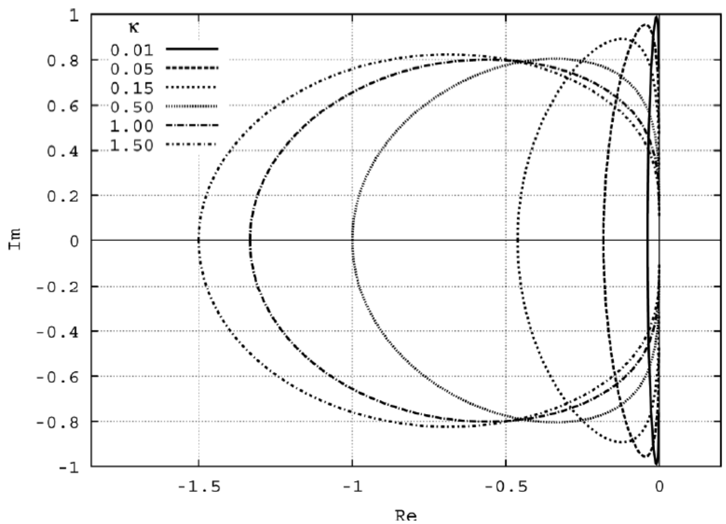
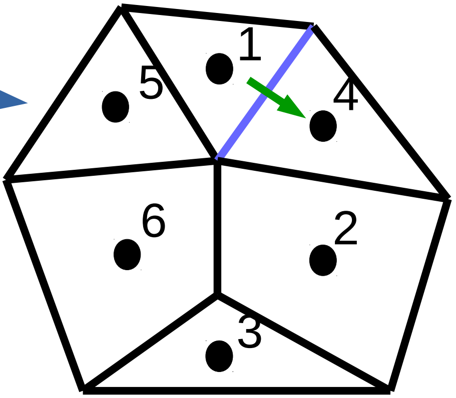


Figure 1 in F.X. Trias and O. Lehmkuhl. “A self-adaptive strategy for the time-integration of Navier-Stokes equations”. Numerical Heat Transfer, part B, 60(2):116–134, 2011.

So, what is **CFL**? A very popular (inaccurate) way to do it

$$\Delta t \leq C_{conv}\left(\frac{\Delta x}{U}\right)_{min} \qquad \Delta t \leq C_{diff}\left(\frac{\Delta x^2}{\nu}\right)_{min}$$

What is Δx and U in an unstructured mesh?



ANSWER: This is the typical "1D uniform mesh" idea applied to "3D unstruct"

$$\boldsymbol{\Omega}\frac{d u_h}{d t}+\boldsymbol{C}(u_h)u_h=\boldsymbol{D}u_h-\boldsymbol{\Omega}\boldsymbol{G}p_h \qquad \boldsymbol{M}u_h=0_h$$

$$-\boldsymbol{C}(u_h)+\boldsymbol{D}$$

Instead we can compute the spectral radius of this operator

REMAINDER!!!

$$u_h^T\boldsymbol{C}(u_h)u_h=0 \longrightarrow \boldsymbol{C}(u_h)=-\boldsymbol{C}^T(u_h)$$

$$u_h^T\boldsymbol{\Omega}\boldsymbol{G}p_h=0 \longrightarrow \boldsymbol{\Omega}\boldsymbol{G}=-\boldsymbol{M}^T$$

$$u_h^T\boldsymbol{D}u_h\leq 0 \longrightarrow \boldsymbol{D}=\boldsymbol{D}^T \text{ def-}$$

Take-away messages

- Many types of pathologies (dispersion&aliasing errors, wiggles,...) are associated with ODD-derivative errors.
- EVEN-derivative errors tend to smooth (diffusion-like process). Hence, they are commonly used (Upwind-like, flux-limiters, filtering, ...) to "heal" our ODD pathologies.

Questions:

- What are the adverse side-effect of these EVEN-derivative healing?
- Is it reasonable to use "1D uniform mesh" ideas for "3D unstructured mesh" problems? Is there a better way to do it?