A general method to compute numerical dispersion error

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1. Numerical Dispersion errors: What are they?
2. Methodology
3. Test cases
4. Conclusions and further work
Some background on numerical errors

Numerical errors are introduced when equations are discretised. Numerical derivatives do not match analytical ones. Numerical Dispersion cannot be avoided, just reduce it. Except if Spectral Methods are used, where derivative is imposed to be exact: $f'(k) = kf(k)$.

How is Numerical Dispersion usually studied? By means of a Fourier Transform.
Numerical Dispersion errors: What are they?

Some background on numerical errors

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- Numerical errors are introduced when equations are discretised.
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  - Numerical errors are introduced when equations are discretised.
- Numerical Diffusion is well known and is easy to eliminate: central or symmetric schemes.
  - If it is not eliminated, the error is proportional to $\Delta x$.
  - Thus, is easy to reduce: densify mesh.
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If a Fourier Transform is used, then just periodic domains with uniform meshes can be studied. The extrapolation to 3D unstructured domains with generic boundary conditions is NOT straightforward. Authors report that conclusions extracted in uniform meshes fail in slightly stretched meshes. Not even unstructured; just stretched. A methodology that allows studying dispersion in a general mesh would be interesting.

Numerical dispersion is, then, a function of the studied mesh. Instead of using the sinusoids base, use an orthogonal base extracted from studied mesh. For example, eigenvectors of the discrete Laplacian matrix.
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- A methodology that allows studying dispersion in a general mesh would be interesting.
  - Numerical dispersion is, then, a function of the studied mesh.
- Instead of using the sinusoids base, use an orthogonal base extracted from studied mesh.
  - For example, eigenvectors of the discrete Laplacian matrix.
Methodology: Calculus background (I)

Let $\Phi = \{\phi_{-N}(x), \phi_{-N+1}(x), \ldots \phi_{-1}(x), \phi_0(x), \phi_1(x), \ldots \phi_N(x)\}$ be an orthonormal basis of functions in a domain $\Omega_x$. 

\[ f(x) \approx S_N = \sum_{m=-N}^{N} \alpha_m \phi_m(x); \lim_{N \to \infty} S_N = f(x). \]
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We can define a mapping $T$

$$ T : \mathcal{L}^2(\Omega_x, x) \mapsto \mathbb{C}^{2N+1}; \quad T : f(x) \mapsto (\alpha_m) \in \mathbb{C}^{2N+1}, $$

where

$$ \alpha_m = \langle f | \phi_m \rangle_{\Omega_x} = \int_{\Omega_x} f(x) \overline{\phi_m(x)} \, dx, \quad (1) $$
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And the inverse mapping of $T$
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We can define a mapping \( T \)

\[
T : \mathcal{L}^2(\Omega_x, x) \mapsto \mathbb{C}^{2N+1}; \quad T : f(x) \mapsto (\alpha_m) \in \mathbb{C}^{2N+1}, \text{ where}
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(1)

And the inverse mapping of \( T \)

\[
T^{-1} : \mathbb{C}^{2N+1} \mapsto \mathcal{L}^2(\Omega_x, x), \quad T : (\alpha_m) \in \mathbb{C}^{2N+1} \mapsto f(x).
\]

\[
f(x) \simeq S_N = \sum_{m=-N}^{N} \alpha_m \phi_m(x); \quad \lim_{N \to \infty} S_N = f(x).
\]

(2)
Methodology: Calculus background (II)

We can write the derivative of \( f(x) \) in terms of the orthonormal basis \( \Phi \):

\[
\frac{df}{dx} \approx S'N = \sum_{m=-N}^{N} \alpha_m \phi'_m(x) \approx \sum_{m=-N}^{N} \gamma_{mn} \phi_n(x),
\]

where \( \gamma_{mn} \) represent the projections of the derivatives of \( \phi_m \) on \( \phi_n \).
Methodology: Calculus background (II)

We can write the derivative of \( f(x) \) in terms of the orthonormal basis \( \Phi \):

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f'(x) \approx S'_N = \sum_{m=-N}^{N} \alpha_m \phi'_m(x) \approx \sum_{m=-N}^{N} \left( \alpha_m \sum_{n=-N}^{N} \gamma_{mn} \phi_n(x) \right), \quad (3)
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We can write the derivative of $f(x)$ in terms of the orthonormal basis $\Phi$:

$$f'(x) \simeq S'_N = \sum_{m=-N}^{N} \alpha_m \phi'_m(x) \simeq \sum_{m=-N}^{N} \left( \alpha_m \sum_{n=-N}^{N} \gamma_{mn} \phi_n(x) \right), \quad (3)$$

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We can define a matrix $\Gamma$

Where its elements $(\Gamma)_{mn} = \gamma_{mn} = \langle \phi'_m | \phi_n \rangle_{\Omega_x}$. The structure of $\Gamma$ will provide information about the errors produced during differentiation.
Numerical Dispersion errors: What are they?
Methodology
Test cases
Conclusions and further work

Calculus background
Algebra background
Orthonormal basis
Phase

Methodology: Calculus background (III)

Some calculus background: Example with sinusoids
Methodology: Calculus background (III)

Some calculus background: Example with sinusoids

If sinusoids ($\phi_m = e^{ik_m x}$) are used as the orthonormal base, such as Fourier Transform does, then matrix $\Gamma$ should be:

$$\Gamma = \text{diag}(k_m) \in \mathcal{I}.$$
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However, three different errors could occur:
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Some calculus background: Example with sinusoids

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- $\gamma_{mn} \neq 0$ if $m \neq n$, 

$\gamma_{mn}$ is the numerical dispersion error coefficient.
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- $\gamma_{mn} \neq 0$ if $m \neq n$,
- $\text{Re}(\gamma_{mm}) \neq 0$, 
- $\text{Im}(\gamma_{mm}) \neq 1$. 

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However, three different errors could occur:

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- \(\text{Re}(\gamma_{mm}) \neq 0\),
- \(\text{Im}(\gamma_{mm}) / k_m \neq 1\),
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Methodology: Algebra background (I)

Hermitian and Skew-Hermitian matrices

Every matrix $A$, for example a discrete differential operator, can be decomposed as the sum of an Hermitian, $D$, plus skew-Hermitian, $C$:

$$C = \frac{1}{2} (A - A^*)$$
$$D = \frac{1}{2} (A + A^*)$$ (4)

Expressing the terms of matrix $\gamma$ in a discrete way, denoted by $\tilde{\gamma}_{mn}$, using aforementioned properties:

$$\tilde{\gamma}_{mn} = \langle A \phi_m | \phi_n \rangle$$ (5)

$$\text{Im} (\tilde{\gamma}_{mn}) = \langle C \phi_m | \phi_n \rangle = \langle A \phi_m | \phi_n \rangle - \langle \phi_m | A \phi_n \rangle$$ (6)

$$\text{Re} (\tilde{\gamma}_{mn}) = \langle D \phi_m | \phi_n \rangle = \langle A \phi_m | \phi_n \rangle + \langle \phi_m | A \phi_n \rangle$$ (7)
Methodology: Algebra background (I)

### Hermitian and Skew-Hermitian matrices

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$$
Methodology: Orthonormal basis

Discrete Laplacian eigenvectors

It is the logical choice. If this has begun with a generalisation of a method that uses Fourier Transform, it's logical to employ the discrete version of what Fourier does: using eigenfunctions of the continuous Laplacian. In evenly spaced domains, i.e. structured uniform meshes, eigenvectors are discretised sinusoids. The set of eigenvectors form an orthonormal base. In the continuous limit, eigenvectors and eigenvalues collapse onto its corresponding eigenfunctions, i.e sinusoids. Retain the concept of mesh connectivity without being restrained to mesh uniformity.
Methodology: Orthonormal basis

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Methodology

Test cases

Conclusions and further work

Calculus background

Algebra background

Orthonormal basis

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Methodology: Orthonormal basis

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Methodology: Eigenvectors example
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Methodology: Phase

Rotation matrix

Sinusoids orthonormal basis have a free parameter: the phase of the function. Working in a discrete way, with eigenvectors, this is translated as a matrix rotation. This allows to obtain the average of the recovered numerical eigenvalue. Useful for non-linear operators or when non-uniform meshes are used. The matrix containing eigenvectors is multiplied by a rotation matrix with a random phase. And this is repeated N times (5000) to ensure a correct average.
Methodology: Phase

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Test cases: Selected cases

Used schemes

- Mixture of linear and non-linear schemes:
  - 2nd and 6th order: \{SP2, SP6\}
  - Dispersion relation preserving of 4th and 6th order: \{DRP4, DRP6\}
  - Moving Least squares of 6th order: \{MLS6\}
  - First-order upwind: \{UPW\}
  - WENO of 3rd, 5th and 7th order: \{WENO3, WENO5, WENO7\}
  - Superbee: \{SB\}
  - Van Leer: \{VL\}
  - Minmod: \{MM\}

Used meshes

Using 30 one-dimensional stretched meshes:
- From 0 to 5% stretching ratio
- \(\Delta x_{\text{min}}\) from 1/32 to 1/512.
Test cases: Selected cases

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Mixture of linear and non-linear schemes:

- Symmetry preserving of $2^{nd}$ and $6^{th}$ order \{SP2, SP6\}
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Test cases: Selected cases

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  - First-order upwind \{UPW\}, WENO of 3\textsuperscript{rd}, 5\textsuperscript{th} and 7\textsuperscript{th} order \{WENO3, WENO5, WENO7\}, and Superbee \{SB\}, Van Leer\{VL\} and Minmod \{MM\} flux limiters.
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### Used schemes

**Mixture of linear and non-linear schemes:**

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### Used meshes

**Using 30 one-dimensional stretched meshes:**

- From 0 to 5% stretching ratio
- $\Delta x_{\text{min}}$ from $1/32$ to $1/512$. 
Test cases: Results

Left: Numerical eigenvalues. Right: Numerical wavenumbers.
Uniform mesh.
Test cases: Results

Left: Numerical eigenvalues. Right: Numerical wavenumbers.

Uniform mesh.

$$\lambda_{an} = \frac{4}{\Delta x} \sin^2 (k_{an}\Delta x)$$
Numerical Dispersion errors: What are they?
Methodology
Test cases
Conclusions and further work

Selected cases
Results
Computational cost

Test cases: Results

Left: Numerical eigenvalues. Right: Numerical wavenumbers.
Until 1% stretching.

\[ \lambda_{\text{num}} \Delta_{\text{Max}} \]
\[ \lambda_{\text{an}} \Delta_{\text{Max}} \]
\[ k_{\text{num}} \Delta_{\text{Max}} \]
\[ k_{\text{an}} \Delta_{\text{Max}} \]
Test cases: Results

Left: Numerical eigenvalues. Right: Numerical wavenumbers. Until 2% stretching.
Test cases: Results

Left: Numerical eigenvalues. Right: Numerical wavenumbers. Until 3% stretching.
Test cases: Results

Left: Numerical eigenvalues. Right: Numerical wavenumbers. Until 4% stretching.
Test cases: Results

Left: Numerical eigenvalues. Right: Numerical wavenumbers.
Until 5% stretching.
Test cases: Results
Numerical Dispersion errors: What are they?

Methodology

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Test cases: Results

![Graphs showing results for different schemes: UPW, DRP4, WENO5]
Test cases: Results
Numerical Dispersion errors: What are they?

**Methodology**

**Test cases**

**Conclusions and further work**

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**Test cases: Results**

Always at $\lambda \Delta x_{Max} = 2$

[Graphs showing results for different cases]
Test cases: Results

Not a clear cut-off k
### Test cases: Results

| Stretch. [%] | SP2   | DRP4   | DRP6   | SP6   | MLS3  |
|--------------|-------|--------|--------|-------|-------|
| 0            | 1     | 1.7254 | 1.8368 | 1.586 | 1.5615|
| 1            | 1.203 | 1.8884 | 1.9638 | 1.7688| 1.7466|
| 2            | 1.2396| 1.8792 | 1.9466 | 1.7704| 1.7488|
| 3            | 1.2501| 1.856  | 1.9239 | 1.7564| 1.7369|
| 4            | 1.2512| 1.8364 | 1.9018 | 1.7412| 1.7205|
| 5            | 1.2432| 1.8223 | 1.8748 | 1.7268| 1.708 |
| AVG          | 1.2374| 1.8565 | 1.9222 | 1.7527| 1.7322|

**Table:** Non-dimensional maximum eigenvalue normalized respect maximum eigenvalue for second-order symmetry preserving in uniform meshes, linear schemes.
Test cases: Results

| Stretch. [%] | SP2     | DRP4    | DRP6    | SP6    | MLS3   |
|-------------|---------|---------|---------|--------|--------|
| 0           | 1       | 1.7254  | 1.8368  | 1.586  | 1.5615 |
| 1           | 1.203   | 1.8884  | 1.9638  | 1.7688 | 1.7466 |
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Test cases: Results

| Stretch. [%] | WENO3 | WENO5 | WENO7 | MM  | SB  | VL  |
|-------------|-------|-------|-------|-----|-----|-----|
| 0           | 1.1667| 1.3317| 1.4529| 1.2526| 1.4053| 1.3237|
| 1           | 1.3747| 1.52  | 1.6315| 1.4713| 1.6272| 1.543 |
| 2           | 1.4036| 1.5402| 1.6432| 1.4946| 1.6444| 1.566 |
| 3           | 1.4072| 1.5362| 1.6377| 1.4966| 1.637  | 1.5611|
| 4           | 1.4047| 1.5296| 1.6249| 1.4973| 1.6344| 1.5573|
| 5           | 1.3889| 1.5183| 1.6132| 1.4736| 1.6205| 1.5374|
| AVG         | 1.3958| 1.5289| 1.6301| 1.4867| 1.6327| 1.553 |

**Table:** Non-dimensional maximum eigenvalue normalized respect maximum eigenvalue for first-order upwind in uniform meshes, non-linear schemes.
### Test cases: Results

| Stretch. [%] | WENO3  | WENO5  | WENO7  | MM     | SB     | VL     |
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Table: Non-dimensional maximum eigenvalue normalized respect maximum eigenvalue for first-order upwind in uniform meshes, non-linear schemes.
Test cases: Computational cost

High-order schemes are more cost-effective. They achieve lesser relative errors than low-order schemes for the same computational cost.
Computational cost vs relative error at uniform meshing.
Test cases: Computational cost

![Graphs showing computational cost vs relative error at uniform meshing.]

At uniform meshing...

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Computational cost vs relative error at 2% stretching.

At slightly stretched...

All schemes present a higher relative error: High-order lose two order of magnitude; low-order just one. High-order schemes seem to have lost order of accuracy. For errors in range, low-order are more cost effective.

J. Ruano, A. Baez Vidal, J. Rigola, F. X. Trias
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Test cases: Computational cost
Numerical Dispersion errors: What are they?

Methodology

Test cases

Conclusions and further work

Test cases: Computational cost

Computational cost vs relative error at 4% stretching

J. Ruano, A. Baez Vidal, J. Rigola, F. X. Trias

A general method to compute numerical dispersion error
Test cases: Computational cost

![Graph showing computational cost vs relative error at 4% stretching.]

At highly stretched...

All schemes relative error is higher than 1%. Non-linear schemes do not behave correctly.
A methodology to compute dispersion error in a general framework has been developed. No mesh uniformity nor periodic boundary conditions are required. Instead, uses the eigenvectors of the discrete Laplacian operator.

A new numerical relation between expected and recovered eigenvalues has been found for studied schemes. Stretched meshes, independently on the stretching factor used on the study range, colapse onto the same plot, which is not the same that if uniform meshes are used.
Conclusions and further work

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A methodology to compute dispersion error in a general framework has been developed.

- No mesh uniformity nor periodic boundary conditions are required. Instead, uses the eigenvectors of the \textit{discrete Laplacian operator}.
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Maximum allowed eigenvalue with minimal dispersion directly related to maximum mesh size ($\lambda \Delta x_{\text{Max}} < 2$).

A maximum allowed frequency related to mesh size does not appear. Instead, results are mesh dependent.

Low-order schemes are less affected with mesh stretching than high-order schemes.

High-order schemes lose order of accuracy whereas low-order seem to keep it.

Further work

Propose a meshing technique leading to dispersion reduction.

Select the most appropriate scheme for a given mesh.
Conclusions and further work

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Thanks for your attention