A general method to compute numerical dispersion error

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Index of Contents

1 Numerical Dispersion errors: What are they?

2 Methodology

3 Test cases

4 Conclusions and further work
Numerical Dispersion errors: What are they?

Some background on numerical errors

Numerical derivatives do not match analytical ones. 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, it is easy to reduce: densify mesh.

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.
Some background on numerical errors

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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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  - 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 \( \Omega_x \).
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We can define a mapping $T$.
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We can define a mapping \( T \)

\[
T : L^2(\Omega_x, x) \mapsto \mathbb{C}^{2N+1}; \quad T : f(x) \mapsto (\alpha_m) \in \mathbb{C}^{2N+1}, \text{ 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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$$\alpha_m = \langle f \mid \phi_m \rangle_{\Omega_x} = \int_{\Omega_x} f(x)\overline{\phi_m(x)} \, dx,$$

(1)

And the inverse mapping of $T$

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

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

(2)
Methodology: Calculus background (II)

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

where $\gamma_{mn}$ represent the projections of the derivatives of $\phi_m$ on $\phi_n$. 

We can define a matrix $\Gamma$ where its elements $(\Gamma)_{mn} = \gamma_{mn} = \langle \phi'_m | \phi_n \rangle$. The structure of $\Gamma$ will provide information about the errors produced during differentiation.
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Methodology: Calculus background (III)

Some calculus background: Example with sinusoids

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Methodology

Test cases

Conclusions and further work

Calculus background

Algebra background

Orthonormal basis

Phase

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A general method to compute numerical dispersion error

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

$$\Gamma = \operatorname{diag}(k_m) \in \mathbb{I}.$$  

However, three different errors could occur:

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

- **Dispersion**
  
  $\operatorname{Re}(\gamma_{mm}) \neq 0$,

- **Difussion**
  
  $\operatorname{Im}(\gamma_{mm}) k_m \neq 1$. 

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However, three different errors could occur:

- **Aliasing**: \( \gamma_{mn} \neq 0 \) if \( m \neq n \).
- **Diffusion**: \( \text{Re}(\gamma_{mm}) \neq 0 \).
- **Dispersion**: \( \text{Im}(\gamma_{mm}) k_m \neq 1 \).
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- $\frac{\text{Im}(\gamma_{mm})}{k_m} \neq 1$, 
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- $\gamma_{mn} \neq 0$ if $m \neq n$, **Aliasing**
- $\text{Re}(\gamma_{mm}) \neq 0$
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Methodology: Algebra background (I)

Hermitian and Skew-Hermitian matrices

\[
\text{Every matrix } A \text{, for example a discrete differential operator, can be decomposed as the sum of an Hermitian, } D, \text{ plus skew-Hermitian, } C:\n
C = \frac{1}{2} (A - A^*) \\
D = \frac{1}{2} (A + A^*) \quad (4)
\]

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

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

\[
\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 \quad (6)
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\[
\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 \quad (7)
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$$ \tilde{\gamma}_{mn} = \langle A\phi_m | \phi_n \rangle $$

$$ Im(\tilde{\gamma}_{mn}) = \langle C\phi_m | \phi_n \rangle = \frac{\langle A\phi_m | \phi_n \rangle - \langle \phi_m | A\phi_n \rangle}{2} $$

$$ Re(\tilde{\gamma}_{mn}) = \langle D\phi_m | \phi_n \rangle = \frac{\langle A\phi_m | \phi_n \rangle + \langle \phi_m | A\phi_n \rangle}{2} $$
Methodology: Orthonormal basis

Discrete Laplacian eigenvectors
Methodology: Orthonormal basis

Discrete Laplacian eigenvectors

- It is the logical choice.
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.
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Discrete Laplacian eigenvectors

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- The set of eigenvectors form an orthonormal base.
Methodology: Orthonormal basis

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- The set of eigenvectors form an orthonormal base.
- In the continuous limit, eigenvectors and eigenvalues colapse onto its corresponding eigenfunctions, i.e sinusoids.
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- The set of eigenvectors form an orthonormal base.

- In the continuous limit, eigenvectors and eigenvalues colapse onto its corresponding eigenfunctions, i.e sinusoids.

- Retain the concept of mesh connectivity without being restrained to mesh uniformity.
Methodology: Eigenvectors example
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Methodology: Phase

Rotation matrix
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.
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- 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.
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.
**Test cases: Selected cases**

### Used schemes

<table>
<thead>
<tr>
<th>Scheme Type</th>
<th>Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mixture of linear and non-linear schemes:</td>
<td></td>
</tr>
<tr>
<td>- Symmetry preserving of 2nd and 6th order</td>
<td></td>
</tr>
<tr>
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<td></td>
</tr>
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<td></td>
</tr>
<tr>
<td>- DRP4, DRP6</td>
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</tr>
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<td>- Moving Least squares of 6th order</td>
<td></td>
</tr>
<tr>
<td>- MLS3</td>
<td></td>
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<td>First-order upwind</td>
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<tr>
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<td>WENO of 3rd, 5th and 7th order</td>
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</tr>
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<td>- WENO3, WENO5, WENO7</td>
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</tr>
<tr>
<td>Superbee</td>
<td></td>
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<tr>
<td>- SB</td>
<td></td>
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<tr>
<td>Van Leer</td>
<td></td>
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<tr>
<td>- VL</td>
<td></td>
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</tr>
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<td></td>
</tr>
</tbody>
</table>

**Used meshes**

Using 30 one-dimensional stretched meshes:

- From 0 to 5% stretching ratio $\Delta x$ min from 1/32 to 1/512.
Test cases: Selected cases

Used schemes

Mixture of linear and non-linear schemes:

- Symmetry preserving of 2nd and 6th order \(\{\text{SP}2, \text{SP}6\}\)
- Dispersion relation preserving of 4th and 6th order \(\{\text{DRP}4, \text{DRP}6\}\)
- Moving Least squares of 6th order \(\{\text{MLS}3\}\)
- First-order upwind \(\{\text{UPW}\}\)
- WENO of 3rd, 5th and 7th order \(\{\text{WENO}3, \text{WENO}5, \text{WENO}7\}\)
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Mixture of linear and non-linear schemes:

- Symmetry preserving of $2^{nd}$ and $6^{th}$ order \{SP2, SP6\}
- Dispersion relation preserving of $4^{th}$ and $6^{th}$ order \{DRP4, DRP6\}, and Moving Least squares of $6^{th}$ order \{MLS3\}
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- First-order upwind \{UPW\}, WENO of $3^{rd}$, $5^{th}$ and $7^{th}$ order \{WENO3, WENO5, WENO7\}, and Superbee \{SB\}, Van Leer\{VL\} and Minmod \{MM\} flux limiters.
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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

Test cases: Results


\[ \lambda_{an} = \frac{4}{\Delta x} \sin^2 (k_{an}\Delta x) \]
Test cases: Results

Until 1% stretching.
Test cases: Results

Test cases: Results

Test cases: Results

Test cases: Results

Test cases: Results
Test cases: Results

- UPW
- DRP4
- WENO5
Test cases: Results
Numerical Dispersion errors: What are they?

Methodology

Test cases

Conclusions and further work

Selected cases

Results

Computational cost

Test cases: Results

Always at $\lambda \Delta x_{\text{Max}} = 2$
Test cases: Results

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

<table>
<thead>
<tr>
<th>Stretch. [%]</th>
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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: Results

<table>
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<tr>
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Test cases: Computational cost

At uniform meshing...

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

Computational cost vs relative error at uniform meshing.
At uniform meshing...

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<th>Methodology</th>
<th>Relative error</th>
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<tr>
<td>SP2DRP4DRP6SP6FVMLS3</td>
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</tr>
<tr>
<td>UPWWENO3WENO5WENO7MMSBVL</td>
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</table>

**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.
Test cases: Computational cost

Computational cost vs relative error at 2% stretching.

J. Ruano, A. Baez Vidal, J. Rigola, F. X. Trias
A general method to compute numerical dispersion error
Test cases: Computational cost

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Test cases: Computational cost

Computational cost vs relative error at 4% stretching
Test cases: Computational cost

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, collapse onto the same plot, which is not the same that if uniform meshes are used.
Conclusions

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**.
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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.
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Thanks for your attention