Algebraic implementation of a flux limiter for heterogeneous computing

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Overview

Portability. Why?

Software

- Legacy codes
- Architecture-dependent
- Non-standard kernels

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Hardware

- New architectures
- Hybrid platforms
- Power consumption

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Challenge

How to design portable/hybrid platform codes?

Portability. How?

Idea

Mathematics are always portable!

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“The reason MATLAB is so good at signal processing is that it was not designed for signal processing. It was designed to do mathematics.“

Jim McClellan
GeorgiaTech

Portability. How?

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May approaching dedicated scientific computing codes from an algebraic perspective help?

Portability. What for?

Casting **computational** operations into **algebraic** forms provides with several advantages:

- fewer number of computing kernels $\rightarrow$ portability
- mathematical formality $\rightarrow$ analysis

Remark[1]

For a typical DNS simulation of an incompressible flow, almost 90% of the operations can be cast into 3 basic kernels:

- `SpMV`
- `DOT`
- `axpy`

[1] Guillermo Oyarzun et al. "Portable implementation model for CFD simulations. Application to hybrid CPU/GPU supercomputers". In: *Int. J. Comut. Fluid Dyn.* 31.9 (2017), pp. 396–411.

Scope

How to design a flux limiter kernel from an algebraic approach?

Advantages

With this approach we aim at:

- High portability
- High degree of abstraction

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Disclaimer

We are not after:

- Discussing Flux Limiters
- Optimize performance

Mathematical Machinery

Algebraic Topology

Your mesh. A starting point.

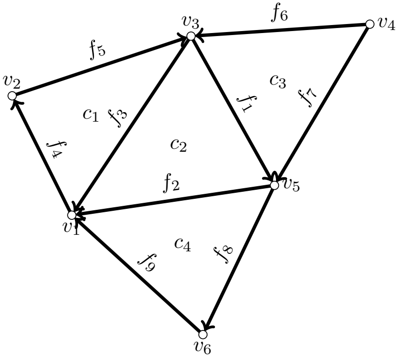


Figure 1: Primal mesh

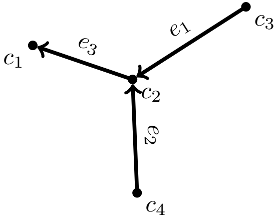
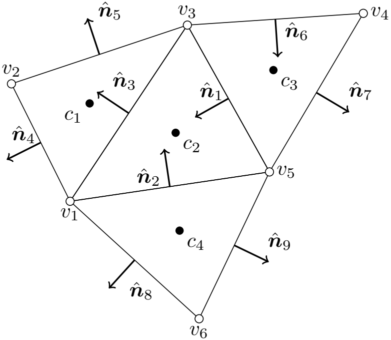


Figure 2: Dual mesh

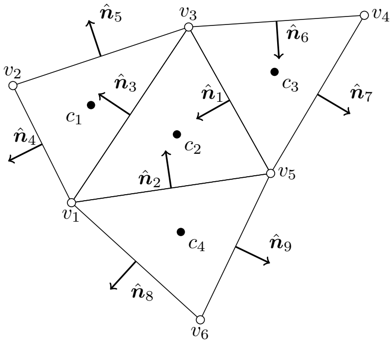
Algebraic Topology



DeRahm Cohomology

$$\begin{array}{ccccccccccc}
\mathbb{R} & \rightarrow & \Lambda_0(\Omega) & \rightarrow & \Lambda_1(\Omega) & \rightarrow & \Lambda_2(\Omega) & \rightarrow & \Lambda_3(\Omega) & \rightarrow & 0 \\
 & & \updownarrow \star & & \updownarrow \star & & \updownarrow \star & & \updownarrow \star & & \\
0 & \leftarrow & \Lambda^3(\Omega) & \leftarrow & \Lambda^2(\Omega) & \leftarrow & \Lambda^1(\Omega) & \leftarrow & \Lambda^0(\Omega) & \leftarrow & \mathbb{R}
\end{array}$$

Algebraic Topology

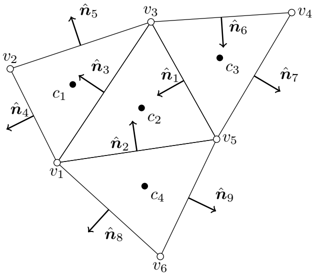


DeRahm Cohomology

Under the hood of:

- Staggered grid
- Symmetry preserving

A graph to rule them all



Operators

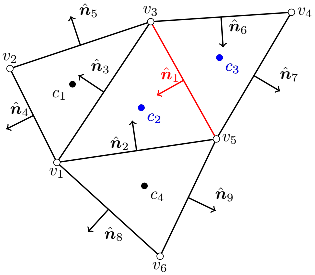
Operators can be constructed from graph information.

$$
T_{cf} = \begin{array}{c} \\ c_1 \\ c_2 \\ c_3 \\ c_4 \end{array}
\begin{array}{c} \begin{array}{ccccccccc} f_1 & f_2 & f_3 & f_4 & f_5 & f_6 & f_7 & f_8 & f_9 \end{array} \\
\begin{pmatrix}
0 & 0 & +1 & -1 & -1 & 0 & 0 & 0 & 0 \\
+1 & +1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & 0 & 0 & 0 & 0 & +1 & -1 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & -1 & -1
\end{pmatrix} \end{array}
$$

A graph to rule them all

Example: Gradient operator

$$\int_{c_3}^{c_2} \nabla P = P_2 - P_3$$



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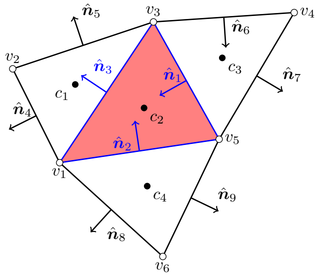
A graph to rule them all

Example: Divergence operator

$$\int_{c_2} \nabla \cdot \vec{u} = \int_{\partial c_2} \vec{u}\hat{n}_f \approx \sum_{f \in c_2} S_f u_f$$



$$T_{cf} = \begin{array}{c} \\ c_1 \\ c_2 \\ c_3 \\ c_4 \end{array} \begin{array}{c} \begin{matrix} f_1 & f_2 & f_3 & f_4 & f_5 & f_6 & f_7 & f_8 & f_9 \end{matrix} \\ \begin{pmatrix} 0 & 0 & +1 & -1 & -1 & 0 & 0 & 0 & 0 \\ +1 & +1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & +1 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & -1 & -1 \end{pmatrix} \end{array}$$

Summary

Metric

Development of numerical method in terms of geometric entities.

$$\Omega_f = \Delta_x S_f$$

Symmetry-preserving

$$GRAD = -\Omega_f^{-1} DIV^T = -(\Delta_x S_f)^{-1} (T_{cf} S_f)^T = -(\Delta_x)^{-1} T_{cf}^T$$

Highlights

- The definition of **star ($\star$)** determines **dual operators**
- Preserve important quantities

Flux Limiters

Flux Limiters

Typically, flux limiters are stated in the following form:

$$\theta_f = \theta_C + \Psi(r)\left(\frac{\theta_D - \theta_U}{2}\right)$$

$$r_f = \frac{\theta_C - \theta_U}{\theta_D - \theta_C} = \frac{\Delta_U \theta_c}{\Delta_u \theta_c}$$

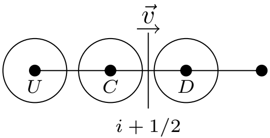


Figure 3: Classical stencil for the computation of the gradient ratio at face $i + 1/2$. U, C and D correspond to the upstream, centered and downstream nodes.

Flux Limiters

Reformulation in terms of matrices [2]

Rearrangement:

$$\theta_f = \frac{\theta_D + \theta_U}{2} + \frac{\Psi(r) - 1}{2} (\theta_D - \theta_U)$$

Matrix formulation:

$$\theta_f = (\Pi_{C \to F} + F(r)_{C \to F})\, \theta_c$$

Dynamic addition of artificial diffusivity as a function of r

[2] F.X. Trias et al. "Symmetry-preserving discretization of Navier–Stokes equations on collocated unstructured grids". In: *J. Comput. Phys.* 258 (Feb. 2014), pp. 246–267.

Gradient Ratio

How to compute the gradient ratio?

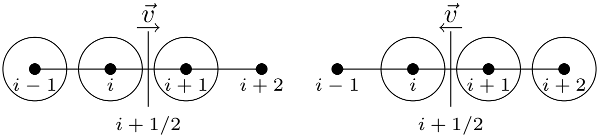


Figure 4: Switched stencil for a typical flux limiter

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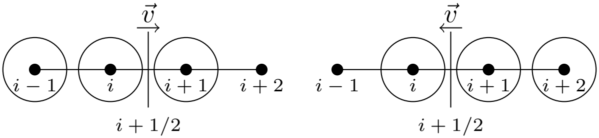

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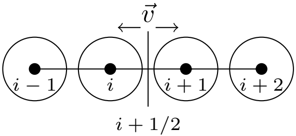

Figure 5: Algebraic stencil for an algebraic flux limiter

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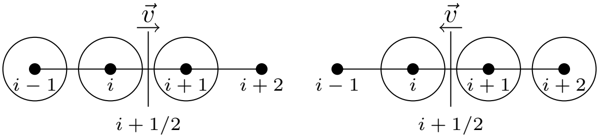

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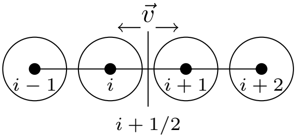

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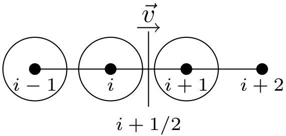

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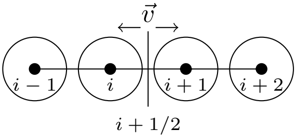

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$$\Delta_u = S(u) T_{cf} \theta_c$$

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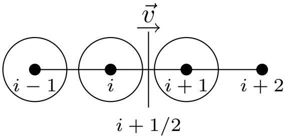

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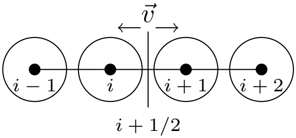

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How to compute Δ_U?

Gradient Ratio

Computing Δ_U

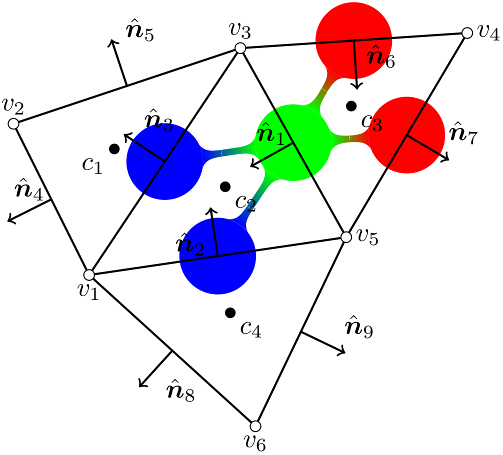
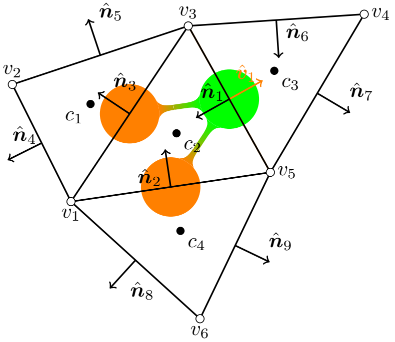


Figure 6: Upstream and Downstream adjacency faces

Gradient Ratio

Idea

1. Vectorize differences
2. Sum up upstream faces
3. Project over the normal



Gradient Ratio

Idea

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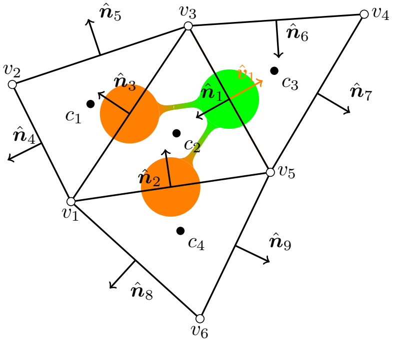
$$\Delta_U = N \left(\mathbb{I}_d \otimes A^U_{FF(u)} \right) N^T \Delta$$



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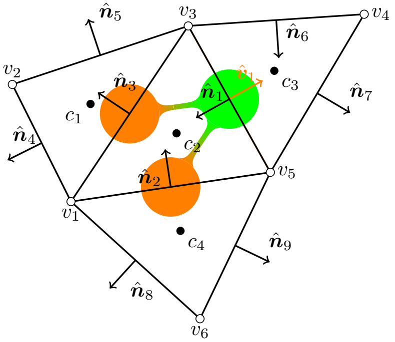
$$N = \begin{pmatrix} n_{1x} & 0 & 0 & n_{1y} & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & n_{9x} & 0 & \dots & n_{9y} \end{pmatrix}$$



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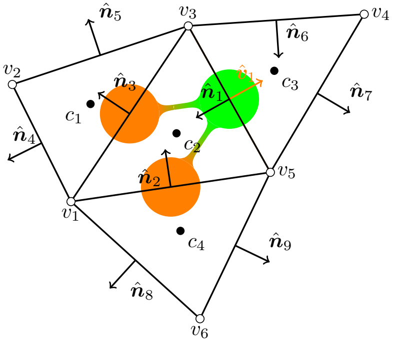
$$A^U_{FF(u)} = \frac{1}{2}\left(S(u)A_{FF} - A^D_{FF}\right)$$



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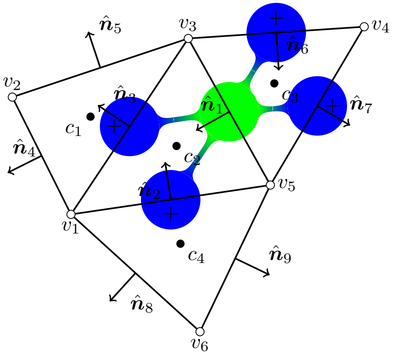

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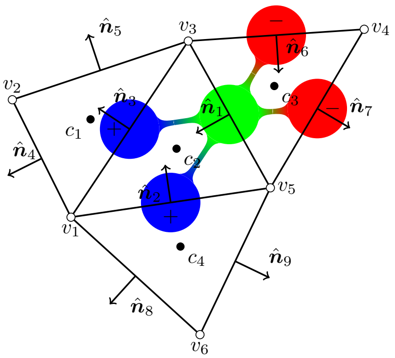

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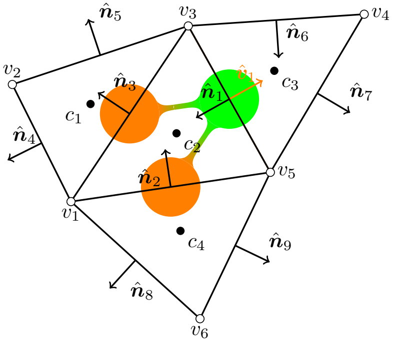


Computational framework

The code has been implemented into HPC^2 - a fully-portable, algebra-based framework for heterogeneous computing [3].

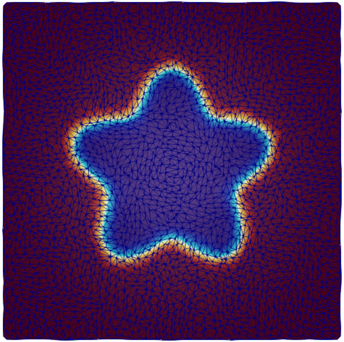
Operation	SpMV	axpy	axdy	shft	scal	vmax vmin	smax smin	sign
$S(u)$	0	0	0	0	0	0	0	1
$\Delta_U\theta$	3	1	0	0	0	0	0	0
$\Delta_u\theta$	2	0	0	0	0	0	0	0
r_f	0	0	1	0	0	0	0	0
$SUPERBEE(r)$	0	0	0	1	1	1	3	0
$F(r)_{C\to F}$	0	0	0	0	1	0	0	0
Euler	6	2	0	0	0	0	0	0
total	11	3	1	1	2	1	3	1

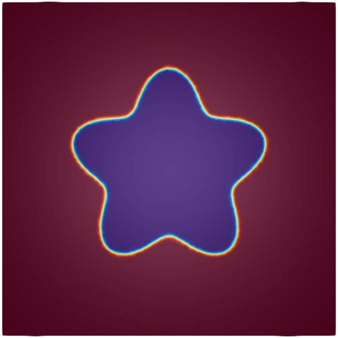
Table 1: Operation count per time step with SUPERBEE and Euler integration [4].

[3] X Álvarez et al. "HPC^2 - a fully-portable, algebra-based framework for heterogeneous computing. Application to CFD". . In: *Comput. Fluids (published online)* (2018).

[4] X Álvarez et al. "Integration of a flux limiter into a fully-portable, algebra-based framework for heterogeneous computing". In: *Tenth Int. Conf. Comput. Fluid Dyn.* Barcelona, 2018.

Advection of a scalar field





Profiles

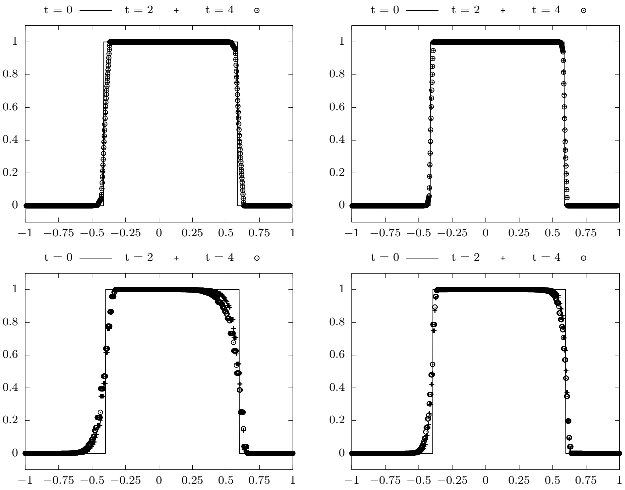


Figure 7: Left column corresponds to a meshes with a characteristic lenght of $\Delta x = 1/32$, while right columns are produced with a characteristic length of $\Delta x = 1/64$.

Conclusions

Highlights

- Flux limiters have been implemented into a portable platform
- Flux limiters **CAN** be cast in an algebraic form
- New conceptual platform developed

Future Work

- Analyze flux limiters properties
- Assess flux limiters design
- Improve gradient reconstruction strategies

Conclusions

Thank you for your attention!