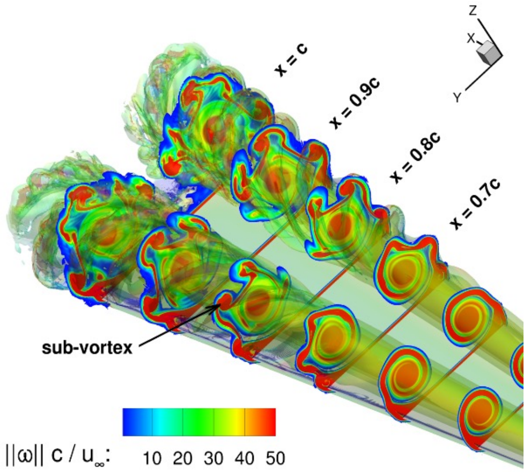

Supraconservative discretization methods for subsonic CFD

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Structure-preserving

Hamiltonian/Poisson	De Rham complex	Invariants
systems & control	differential geometry	conservation laws
dynamical systems	discrete exterior calculus	primary & secondary
symplectic	*mimetic*	*supraconservative*
	(more by Artur Palha)	*(several presentations)*

Invariants & accuracy

Problem: For many industrial flow problems computers are still too slow

Challenge: Get more accuracy from affordable, coarse grids (no theory known)

Observation: Preserving (primary & secondary) invariants can help:
- energy-preserving methods for long-term weather prediction (1960s)
- finite-volume methods for shock waves (1970s - 1980s)

Goal: Preserve some of the invariants after discretization
→ (supra)conservative methods

Application: Physical flow disturbances and instabilities:
e.g. turbulent flow, acoustics, breaking waves, …

Supraconservative choices

Application

incompressible / compressible (shock waves) / multiphase / shallow-water / …

Invariants?

mass, (linear / angular) momentum, (kinetic + internal = total) energy, helicity,
circulation (Kelvin), pressure equilibrium, dispersion relation, time reversibility, …
2D: integrals of vorticity (enstrophy, …)

Basic variables?

primitive variables / streamfunction-vorticity / velocity-vorticity / √ρ-vars / entropy vars / …

Analytical form?

advective / conservative / rotational / split forms / Jacobians / Hamiltonian / variational / …

Computational grid?

collocated / staggered, (non)uniform / curvilinear / unstructured, particles, …

Discretization method?

finite-differences / -elements / -volumes, spectral, compact, mimetic, LB/SPH/…

Some secondary-preservation pioneers

Incompressible Navier–Stokes

1959	Phillips* (387 cits)†	advective	FD	non-linear instability
1966	Arakawa* (2433 cits)	streamf^n-vorticity	FD	kin. energy (KE), enstrophy, curvilinear
1966	Bryan* (123 cits)	conservative	FV	Ma, Mom, KE, non-uniform
1970	Piacsek (365 cits)	skew-symmetric	FD	KE
1987	Horiuti (148 cits)	rotational	FD	KE
1994	Strand (850 cits)	advective	SBP	KE
97/03	Verstappen (135/820 cits)	conservative	FV	Ma, Mom, KE, higher-order non-uniform
2000	Perot (369 cits)	rotational	FD	KE, unstructured staggered
2004	Morinishi (176 cits)	skew-symmetric	FD	KE, curvilinear
2004	Liu/Wang (71 cits)	Jacobians	FD	KE, helicity
2007	Götze (151 cits)	particle model	MPC	angular momentum
2007	Rebholz (68 cits)	variational form	FE	KE, helicity
2014	Trias (205 cits)	conservative	FV	Ma, Mom, KE, unstructured collocated
2017	Palha (104 cits)	rotational-vorticity	FE	Ma, KE, enstrophy, vorticity, reversibility
2017	Charnyi (172 cits)	EMAC form	FE	(Ang)Mom, KE, helicity, enstrophy, vorticity
2021	Komen (52 cits)	conservative	FV	KE, OpenFOAM

*) Long-term weather prediction

†) # Google Scholar citations as of 27 December 2025

‘Ansatz’

How to order this ‘jungle’ of approaches?

Go discrete !

Example: Preservation of energy

Conservation

$$\frac{\partial \phi}{\partial t} + \nabla \cdot \boldsymbol{f}(\phi) = 0, \qquad \boldsymbol{f} \text{ flux function}$$

Finite-volume discretization ($\mathfrak{H}$ control volume; ignore boundary effects)

$$\int_{\mathfrak{H}} \frac{\mathrm{d}\phi}{\mathrm{d}t}\,\mathrm{d}\mathfrak{H} + \int_{\Gamma_{\mathfrak{H}}} \boldsymbol{n} \cdot \boldsymbol{f}(\phi)\,\mathrm{d}\Gamma_{\mathfrak{H}} = 0 \quad \Rightarrow \quad \boxed{\mathfrak{H}\frac{\mathrm{d}\boldsymbol{\phi}}{\mathrm{d}t} + \mathfrak{D}\mathsf{f}(\boldsymbol{\phi}) = 0}$$

$\mathfrak{H}$ diagonal matrix with sizes of grid cells (but may be more general)

- Volume-consistent scaling $\leftrightarrow$ quadrature rule ($\mathbf{1}$ is all-ones vector)

$$\mathbf{1}^{\mathsf{T}}\mathfrak{H}\boldsymbol{\phi} = \sum_{\text{cells}} \mathfrak{H}\boldsymbol{\phi} \approx \int_{\boldsymbol{\Omega}} \phi\,\mathrm{d}\boldsymbol{\Omega} \quad (\forall \phi)$$

$$\int_{\Omega} \frac{\partial \phi}{\partial t}\,\mathrm{d}\Omega = 0 \leftrightarrow \mathbf{1}^{\mathsf{T}}\mathfrak{H}\frac{\mathrm{d}\boldsymbol{\phi}}{\mathrm{d}t} = 0 \;\Leftrightarrow\; \mathbf{1}^{\mathsf{T}}\mathfrak{D}\mathsf{f}(\boldsymbol{\phi}) = 0\;\forall\,\boldsymbol{\phi} \;\Leftrightarrow\; \mathbf{1}^{\mathsf{T}}\mathfrak{D} = \mathbf{0}^{\mathsf{T}}$$

$\Rightarrow$ *Global conservation is equivalent with vanishing column sums*

Discrete equations

E.g. finite-volume formulation ('usually' $\boldsymbol{m} = \rho \boldsymbol{u}$)

$$\int_{\Omega_h} \frac{\partial \rho \psi}{\partial t} \, \mathrm{d}\Omega_h + \int_{\Gamma_h} (\boldsymbol{m} \cdot \boldsymbol{n}) \psi \, \mathrm{d}\Gamma_h = \ldots, \qquad \psi \in \{1, \boldsymbol{u}, e\},$$

but any other origin of the discrete equations is allowed !

mass	$\mathfrak{H} \dfrac{\partial \rho}{\partial t} + \mathfrak{D}_{\mathrm{mass}} \, \boldsymbol{m} = 0$
momentum	$\mathfrak{H} \dfrac{\partial \rho \boldsymbol{u}}{\partial t} + \mathfrak{C}^{m}_{\mathrm{mom}} \, \boldsymbol{u} = -\mathfrak{G}_{\mathrm{mom}} \, p$
int. energy	$\mathfrak{H} \dfrac{\partial \rho e}{\partial t} + \mathfrak{C}^{m}_{\mathrm{inten}} e = -p \, \mathfrak{D}_{\mathrm{inten}} \, \boldsymbol{u}$

$\mathfrak{H}$ is size of control volumes, i.e. *volume-consistent* scaling

Conservation of energy

$$\frac{\partial}{\partial t}(\rho E_{\text{tot}}) = -\frac{1}{2}(\boldsymbol{u}\cdot\boldsymbol{u})\frac{\partial}{\partial t}\rho + \boldsymbol{u}\cdot\frac{\partial}{\partial t}(\rho\boldsymbol{u}) + \frac{\partial}{\partial t}(\rho e)$$

$$= \overbrace{\frac{1}{2}(\boldsymbol{u}\cdot\boldsymbol{u})\nabla\cdot\boldsymbol{m}}^{\text{mass}} - \boldsymbol{u}\cdot\overbrace{\left\{\nabla\cdot(\boldsymbol{m}\otimes\boldsymbol{u}) + \nabla p\right\}}^{\text{momentum}} - \overbrace{\left\{\nabla\cdot(\boldsymbol{m}e) + p\nabla\cdot\boldsymbol{u}\right\}}^{\text{internal energy}}$$

$$= \underbrace{\boldsymbol{u}\cdot\left\{\frac{1}{2}(\nabla\cdot\boldsymbol{m})\boldsymbol{u} - \nabla\cdot(\boldsymbol{m}\otimes\boldsymbol{u})\right\}}_{\text{Property 1}} - \nabla\cdot(\boldsymbol{m}e) - \underbrace{\left\{\boldsymbol{u}\cdot\nabla p + p\nabla\cdot\boldsymbol{u}\right\}}_{\text{Property 2}}$$

$$= \underbrace{-\nabla\cdot(\tfrac{1}{2}\boldsymbol{m}u^2) - \nabla\cdot(\boldsymbol{m}e)}_{\text{Property 3}} - \nabla\cdot(p\boldsymbol{u})$$

$$= -\nabla\cdot(\boldsymbol{m}E_{\text{tot}}) - \nabla\cdot(p\boldsymbol{u})$$

Evolution of discrete energy

$$\frac{\partial}{\partial t}\sum_{\Omega_h}\mathfrak{H}(\rho E_{\text{total}}) = -\sum_{\Omega_h}\boldsymbol{u}\cdot\overbrace{\left(\mathfrak{C}^{m}_{\text{mom}} - \tfrac{1}{2}\,\mathsf{diag}(\mathfrak{D}_{\text{mass}}\boldsymbol{m})\right)}^{\mathfrak{A}_{\text{kin}}}\boldsymbol{u}$$

$$-\sum_{\Omega_h}\left(\boldsymbol{u}\cdot\mathfrak{G}_{\text{mom}}p + p\,\mathfrak{D}_{\text{inten}}\boldsymbol{u}\right) - \sum_{\Omega_h}\mathfrak{C}^{m}_{\text{inten}}e$$

Sufficient (Req 1-3) and necessary (Req 1 and Req 2) conditions for energy preservation (a.k.a. L_2-norm):

$\mathsf{Req}^{\text{mt}}\ 1 \quad \Rightarrow \quad \mathfrak{A}_{\text{kin}} \equiv \mathfrak{C}^{m}_{\text{mom}} - \frac{1}{2}\,\mathsf{diag}(\mathfrak{D}_{\text{mass}}\boldsymbol{m})$ *is skew-symmetric*

$\mathsf{Req}^{\text{mt}}\ 2 \quad \Rightarrow \quad \mathfrak{G}_{\text{mom}} = -\mathfrak{D}^{T}_{\text{inten}} \overset{(*)}{=} -\mathfrak{D}^{T}_{\text{mass}}$ $\quad {}^{(*)}$ incompr. limit

$\mathsf{Req}^{\text{mt}}\ 3 \quad \Rightarrow \quad \mathfrak{C}^{m}_{\text{inten}} = \mathfrak{C}^{m}_{\text{mom}}$

Discrete convection determines all other terms

Mass flux $\boldsymbol{m} \approx \rho\boldsymbol{u}$ is arbitrary - gives large freedom

AEPV, J. Comput. Phys. 398:108894 (2019); SIAM Review 63:756-779 (2021)

Freedom in mass flux

Face interpolations between cell c *and neighbor* nb	mass flux $\boldsymbol{m}_{\text{face}} \approx \rho \boldsymbol{u}$
split forms [1]*:*	
Feiereisen (1981); Kok (2009); Kuya (2018)	$\frac{1}{2}(\rho_{\text{c}}\boldsymbol{u}_{\text{c}} + \rho_{\text{nb}}\boldsymbol{u}_{\text{nb}})$
Kennedy/Gruber (2008); Pirozzoli (2010); Kuya (2018)	$\frac{1}{4}(\rho_{\text{c}} + \rho_{\text{nb}})(\boldsymbol{u}_{\text{c}} + \boldsymbol{u}_{\text{nb}})$
Coppola (2019)	$\frac{1}{2}(\rho_{\text{c}}\boldsymbol{u}_{\text{nb}} + \rho_{\text{nb}}\boldsymbol{u}_{\text{c}})$
logarithmic fluxes (for shocks [2]*):*	
Chandrashekar (2013); Ranocha (2018, 2020)	$\dfrac{\rho_{\text{nb}} - \rho_{\text{c}}}{\ln \rho_{\text{nb}} - \ln \rho_{\text{c}}}(\boldsymbol{u}_{\text{c}} + \boldsymbol{u}_{\text{nb}})$
$\sqrt{\rho}$*-variables (allow symplectic time integration* [3]*):*	
Subbareddy (2009); Reiss (2014); Rozema (2014)	$\frac{1}{2}\sqrt{\rho_{\text{c}}}\sqrt{\rho_{\text{nb}}}(\boldsymbol{u}_{\text{c}} + \boldsymbol{u}_{\text{nb}})$

[1] More about split forms by Gennaro Coppola

[2] More about shocks by Sergio Pirozzoli and Henrik Ranocha

[3] More about time integration by Francesco Capuano

‘Convective’ summary

Discrete equations with volume-consistent scaling

$$\text{mass:}\quad \mathfrak{H}\frac{\mathrm{d}\rho}{\mathrm{d}t} + \mathfrak{D}_{\text{mass}}\mathsf{m} = 0; \qquad \text{momentum:}\quad \mathfrak{H}\frac{\mathrm{d}\rho\phi}{\mathrm{d}t} + \mathfrak{C}^{m}_{\text{mom}}\phi = 0$$

conserved	*necessary & sufficient*		*necessary*
mass	$\mathbf{1}^T\mathfrak{D}_{\text{mass}} = \mathbf{0}$		
momentum	$\mathbf{1}^{\mathbf{T}}\mathfrak{C}^{m}_{\text{mom}} = \mathbf{0}$	$\Rightarrow$	$\mathfrak{D}_{\text{mass}}\mathsf{m} = \mathfrak{C}^{m}_{\text{mom}}\mathbf{1}$
energy	$\mathfrak{C}^{m}_{\text{mom}} - \frac{1}{2}\,\mathrm{diag}(\mathfrak{D}_{\text{mass}}\mathsf{m})$ skew-symmetric		$\rightarrow$ mass conservation

Discrete conservation of momentum and energy $\Rightarrow$ conservation of mass

Non-interference

Each physical phenomenon has its own ‘action’

- *Convection* moves ‘stuff’ from A to B; does not change anything
  - Linear algebra → eigenvalues purely imaginary = close to instability
  - “Non-linear instability” is a misnomer (Bryan also knew this in 1966)
- *Pressure* does work only by compression
- For incompressible flow, only *viscosity* dissipates energy
- *Shock waves* also dissipate energy (compression, entropy, viscosity)

Principle of non-interference

Above properties should also hold after discretization

Discretizations

Linear algebra and conservation

- Shift operator (1-dim) $\mathsf{E}(\phi)|_i = \phi_{i+1}$:

$$\text{Finite-volume} \quad \Rightarrow \quad \mathfrak{D} = \mathsf{E} - \mathsf{I} \leftrightarrow \mathfrak{H}\frac{\mathrm{d}\phi}{\mathrm{d}t} + (\mathsf{E} - \mathsf{I})\mathsf{f}(\phi) = 0$$

- Matrix decomposition:

*Lemma**: Any matrix $\mathfrak{D}$ with vanishing column sums, i.e. $\mathbf{1}^{\mathsf{T}}\mathfrak{D} = \mathbf{0}^{\mathsf{T}}$, can be decomposed as

$$\mathfrak{D} = (\mathsf{E} - \mathsf{I})\mathfrak{F} \quad \text{for some flux matrix } \mathfrak{F}$$

$\Rightarrow$ Any conservative discretization can be written as a finite-volume discretization

The converse, i.e. whether any FV discretization can be written as a FD discretization for a creatively constructed analytic PDE form, is still an open question
More about such a possible converse by Gennaro Coppola

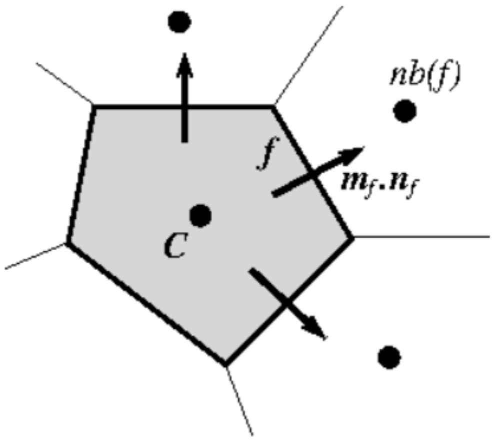
*) G. Coppola & AEPV, J. Comput. Phys. 475:111879 (2023)

Finite volume: collocated, unstructured

Discrete conservation of mass and momentum

$$\mathfrak{H}\frac{\partial \rho}{\partial t} + \sum_{f\in\mathcal{F}_C} (\boldsymbol{m}\cdot\boldsymbol{n})_f \,\mathrm{d}\Gamma_f = 0; \qquad \mathfrak{H}\frac{\partial \rho\phi}{\partial t} + \sum_{f\in\mathcal{F}_C} (\boldsymbol{m}\cdot\boldsymbol{n})_f \phi_f \,\mathrm{d}\Gamma_f = 0$$

- Skew symmetry determines several details:



Off diagonal Flux ϕ_f must be symmetric

$$\phi_f = \tfrac{1}{2}(\phi_C + \phi_{nb(f)})$$

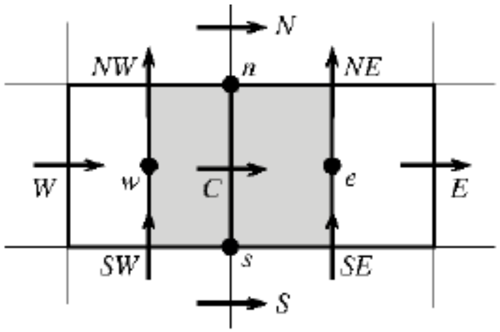
irrespective of geometry

Diagonal Fixes discrete divergence operator $\mathfrak{D}_{\mathrm{mass}}$

$$\mathfrak{D}_{\mathrm{mass}}\boldsymbol{m}|_C = 2\,\mathrm{diag}(\mathfrak{C}^m_{\mathrm{mom}})|_C = \sum_{f\in\mathcal{F}_C} (\boldsymbol{m}\cdot\boldsymbol{n})_f \,\mathrm{d}\Gamma_f$$

$=$ natural for FV; still no restrictions on mass flux $\boldsymbol{m}_f$

FV: staggered, structured



Mass (right basic cell)

$$\mathfrak{D}_{\mathrm{mass}}\,\mathsf{m}|_e = m^x_E + m^y_{NE} - m^x_C - m^y_{SE}$$

Convection (shaded cell)

$$\begin{aligned}\mathfrak{C}^m_{\mathrm{mom}}\,\mathsf{u}_x|_C &= m^x_e\,u_e + m^y_n\,u_n - m^x_w\,u_w - m^y_s\,u_s \\ &= \tfrac{1}{2}[m^x_e u_E - m^x_w u_W + m^y_n u_N - m^y_s u_S] + \tfrac{1}{2}[m^x_e - m^x_w + m^y_n - m^y_s]u_C\end{aligned}$$

Coefficient of u_C vanishes ($= \frac{1}{2}$ mass flux for two basic cells)

Pressure gradient incompressible $\rightarrow$ Poisson equation

$$0 = \frac{\partial}{\partial t}\mathfrak{D}_{\mathrm{mass}}\,\mathsf{m} \overset{(*)}{=} \mathfrak{D}_{\mathrm{mass}}\frac{\partial \rho\mathsf{u}}{\partial t} = -\mathfrak{D}_{\mathrm{mass}}\,\mathfrak{H}^{-1}\left(\mathfrak{C}^m_{\mathrm{mom}}\,\mathsf{u} + \mathfrak{G}_{\mathrm{mom}}\,p\right)$$

Step (*) is only place where $\mathsf{m} = \rho\mathsf{u}$ is needed

In general: Same interpolation for staggered momentum quantities $\mathfrak{H}$, ρ, m, u, $\mathfrak{C}^m_{\mathrm{mom}}$, $\mathfrak{D}_{\mathrm{mass}}$

More about staggered discretization by Xavi Trias

Higher order

- *Higher-order barrier*[1)]
  Mass fluxes of a single term $\mathsf{m}_f \phi_f$ can be at most second-order accurate

- *Structured grids*
  E.g., Richardson extrapolation from fine grid and 2× coarser grid[2)] :

$$\mathfrak{H}^{4\text{th}} = (8\,\mathfrak{H}^{\text{fine}} - \mathfrak{H}^{\text{crse}})/6 \quad \text{(Simpson quadrature rule)}$$

$$\mathfrak{C}^{4\text{th}}_{\text{mom}} = (8\,\mathfrak{C}^{\text{fine}}_{\text{mom}} - \mathfrak{C}^{\text{crse}}_{\text{mom}})/6$$

$$\mathfrak{C}^{\text{fine}}_{\text{mom}}\phi = \tfrac{1}{2}(\mathsf{I} - \mathsf{E}^{-1})\,\mathsf{M}^{\text{fine}}_f\,(\mathsf{I} + \mathsf{E})\phi \quad \text{with} \quad \mathsf{M}^{\text{fine}}_f = \tfrac{1}{2}\,\text{diag}[(\mathsf{I} + \mathsf{E})\mathsf{m}]$$

$$\mathfrak{C}^{\text{crse}}_{\text{mom}}\phi = \tfrac{1}{2}(\mathsf{I} - \mathsf{E}^{-2})\,\mathsf{M}^{\text{crse}}_f\,(\mathsf{I} + \mathsf{E}^2)\phi \quad \text{with} \quad \mathsf{M}^{\text{crse}}_f = \tfrac{1}{2}\,\text{diag}[(\mathsf{I} + \mathsf{E}^2)\mathsf{m}]$$

  The resulting 4^{th}-order mass flux equals[3)]

$$(m\phi)^{4\text{th}}_{i+1/2} = \frac{1}{6}\left[8\left(\frac{m_{i+1}+m_i}{2}\right)\left(\frac{\phi_{i+1}+\phi_i}{2}\right) - \left(\frac{m_{i+2}+m_i}{2}\right)\left(\frac{\phi_{i+2}+\phi_i}{2}\right) - \left(\frac{m_{i+1}+m_{i-1}}{2}\right)\left(\frac{\phi_{i+1}+\phi_{i-1}}{2}\right)\right]$$

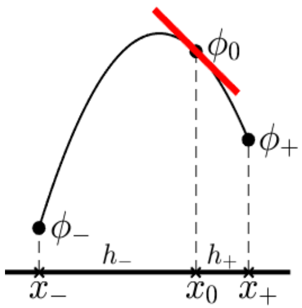
- *Unstructured grids*
  Higher-order methods still open - FEM can give ideas

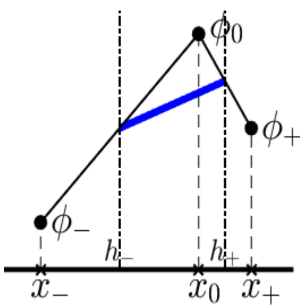
1) G. Coppola & AEPV, J. Comput. Phys. 475:111879 (2023)
2) R. Verstappen & AEPV, J. Comput. Phys. 187:343–368 (2003)
3) S. Pirozzoli, J. Comput. Phys. 229(19):7180–7190 (2010)

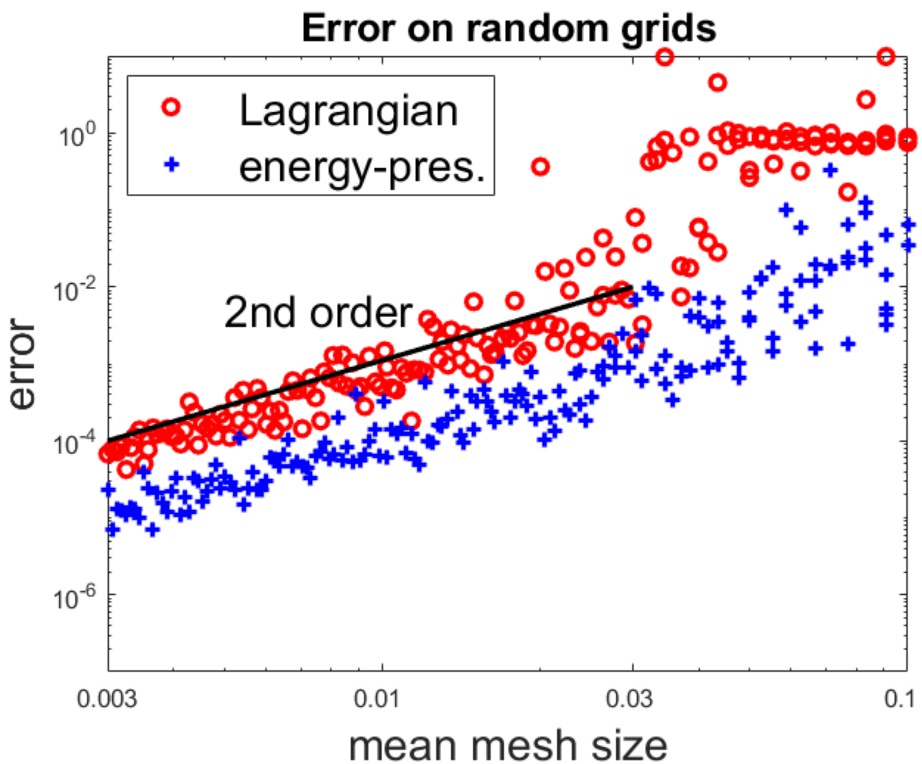
Simulations on coarse grids

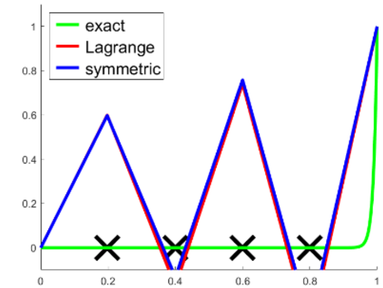
ConvDiff - random exponential grids

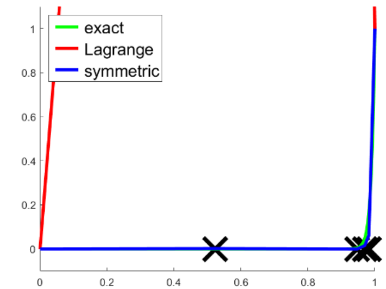
$$\frac{\mathrm{d}\phi}{\mathrm{d}x} - \mu \frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} = 0, \;\; \mu = 0.01$$

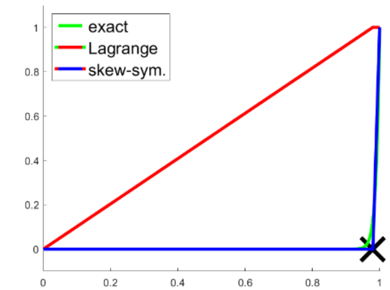












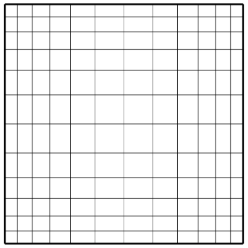
See also: E. Dobelis, A Comparison of Discretization Methods on Coarse Non-Uniform Grids, BSc thesis, RUG, June2025

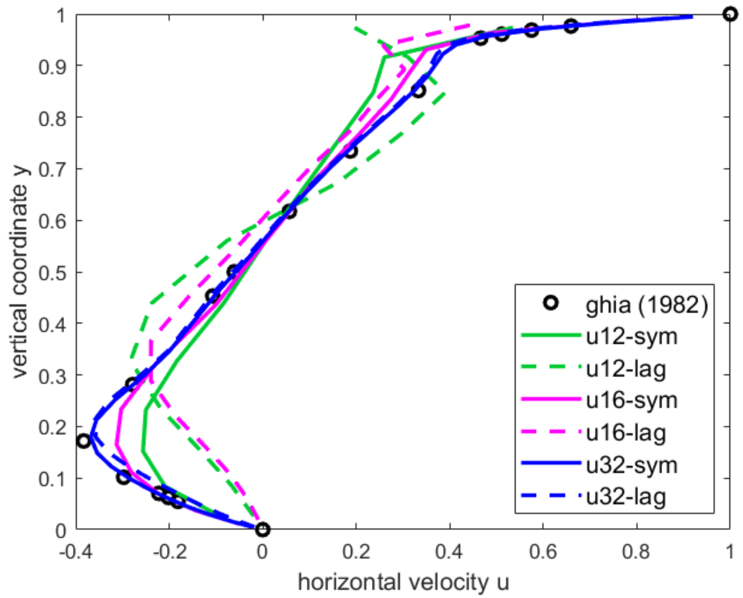
Driven cavity

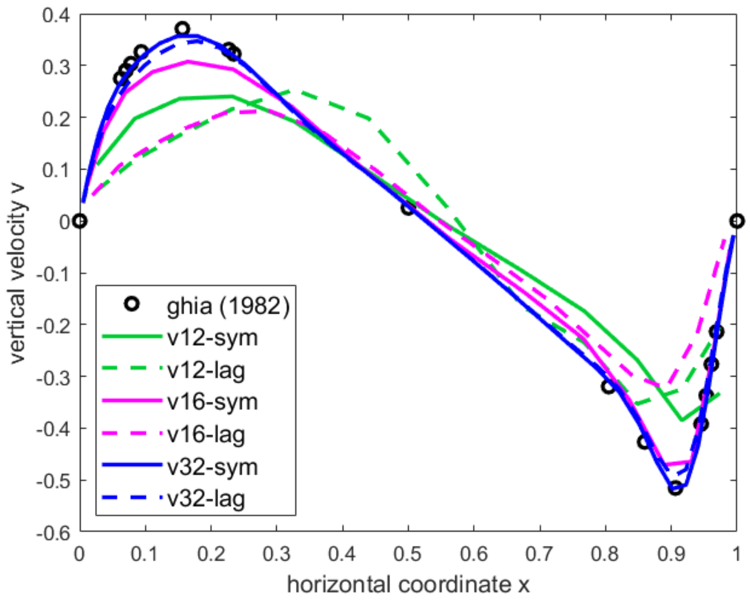
Driven cavity Re=100 – centerline velocities

non-uniform grids 12x12, 16x16, 32x32

12 x 12 grid







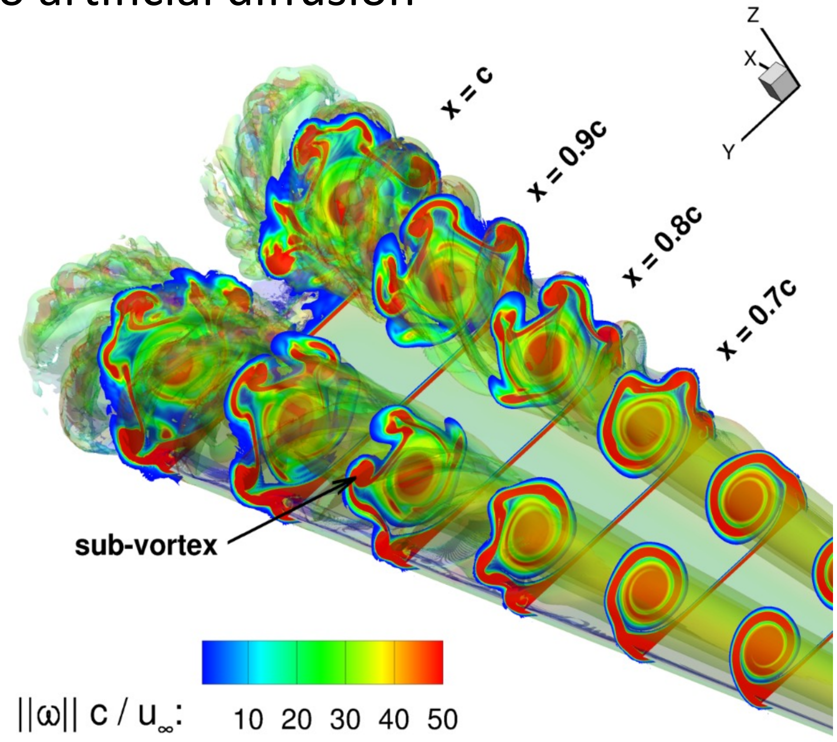
Skew-symmetric (———) versus Lagrangian (– – – –) central discretization

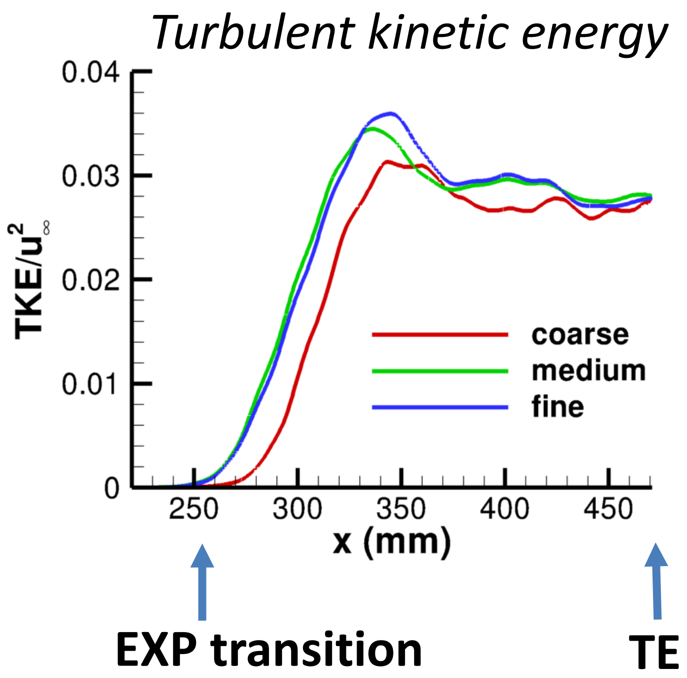
Delta wing: compressible flow

Subsonic flow past delta wing at Re_c=150,000 : DNS vs. experiment

Natural laminar-turbulent transition

No artificial diffusion



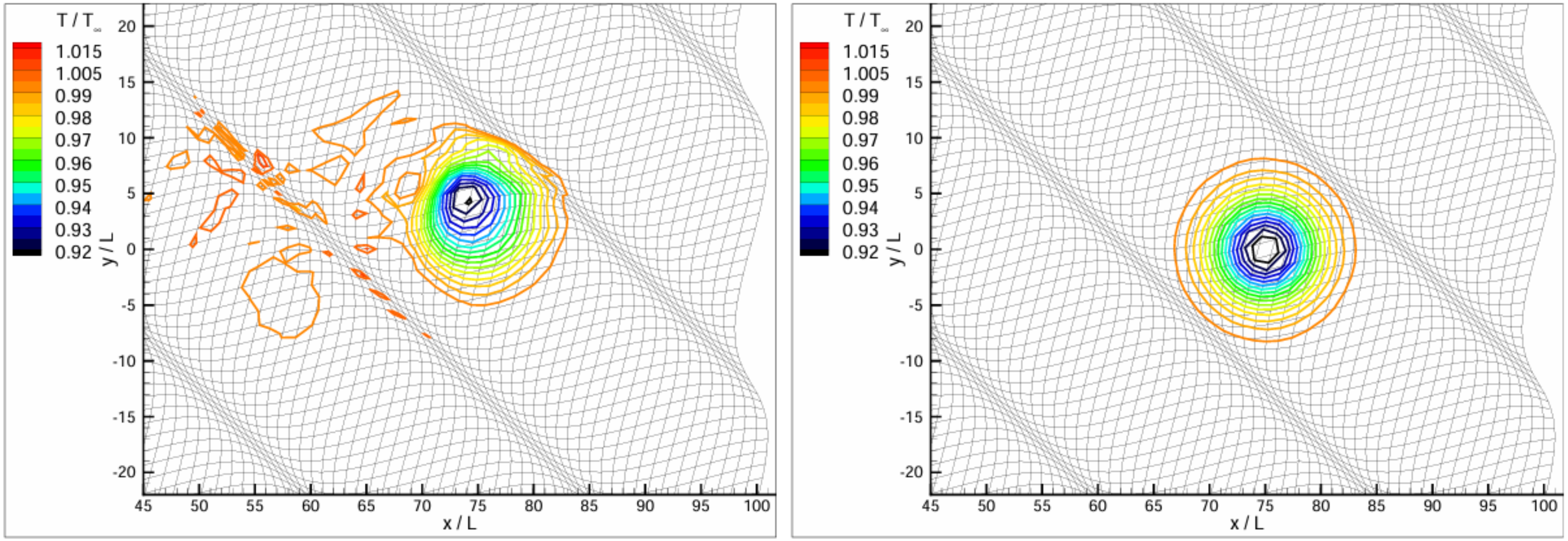


W. Rozema, et al. J. Comput. Phys. 405:109182 (2020)

Acoustics (Euler)

Convection of isotropic vortex in uniform flow - Mach = 0.5

Preserves kinetic energy and dispersion relation - 'supra^{2}conservative'



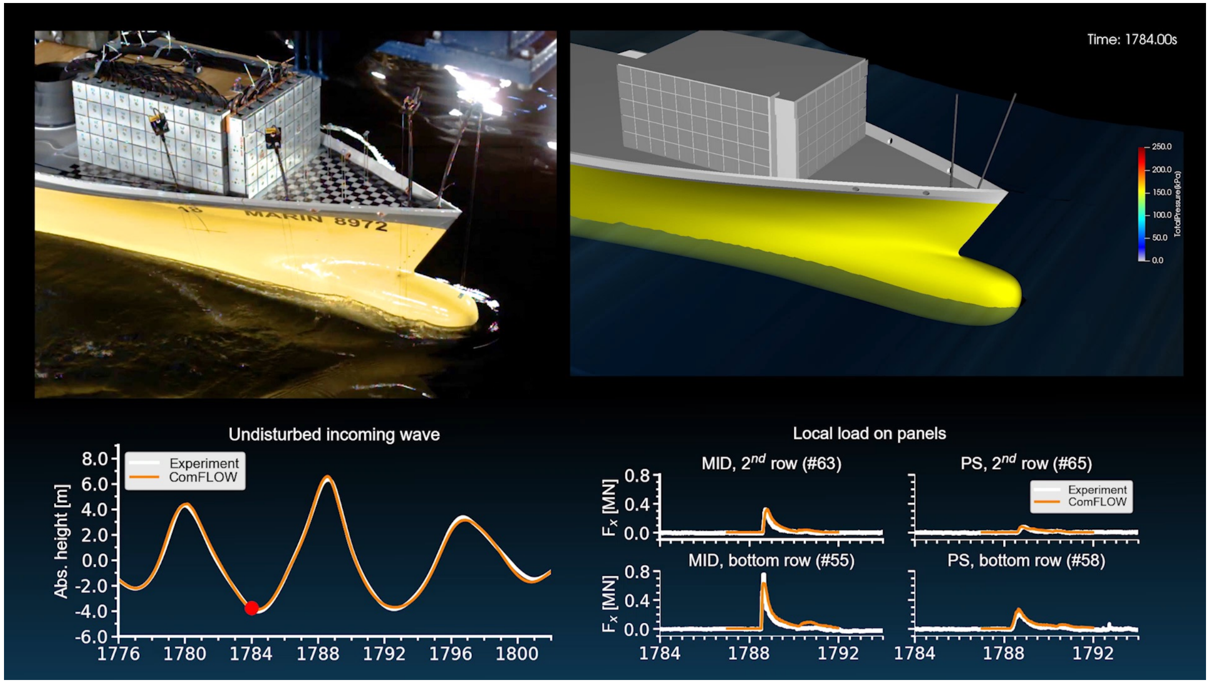
Standard non-symmetric discretization *Skew-symmetric discretization*

J.C. Kok, J. Comput. Phys. 228:6811-6832 (2009)

Multiphase flow

Instabilities at tips of breaking waves

Exchange between kinetic, potential and capillary energy



R.A. Remmerswaal, arXiv:2209.14934 (2022); PhD thesis, Univ. Groningen, 2023

Conclusions

Supraconservative discretization of subsonic NS

- Discussion at discrete level, independent of analytical origin
- FV helps to reduce the 'jungle' of secondary-preserving discretizations
- Necessary and sufficient conditions for energy preservation
  - Discrete convection determines all other terms except diffusion
  - Mass fluxes arbitrary; momentum fluxes ½ - ½ interpolation
- For incompressible flow, provably stable without artificial diffusion
- Forgiving to irregular, coarse grids – more theory desired

Research themes

- How to combine this philosophy with turbulence modelling?

  More by Andrea Beck, Benjamin Sanderse and Roel Verstappen

- How to combine analysis with (energy dissipating) shock waves?

  More by Francesco Capuano, Gennaro Coppola and Sergio Pirozolli

- How to design higher-order variants for unstructured grids?

  More by Oriol Lehmkuhl and Xavi Trias

- How to combine geometric flexibility of FEM with supraconservation of FVM?

  More by Alessandro Colombo and Artur Palha

- Which secondary invariant is most suited for a given application on coarse grids, and can it be analysed in a similar way ?

- What does this approach imply for the Jacobian matrix (bifurcations)?

- How to transfer new CFD approaches to industrial software?

  More by Pedro Costa, Ed Komen, Henrik Ranocha and Francesc Verdugo