





Quelques intégrateurs géométriques

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Geometric integrator

Discretization scheme which respects *exactly* some geometric properties



Invariant integrator

Symmetry group

- Differential equation: $E(\mathbf{x}, \mathbf{u}, \mathbf{u}_{(1)}, \ldots) = 0$
- ► Transformation $(\mathbf{x}, \mathbf{u}) \mapsto (\hat{x}, \hat{u})$ is a symmetry if $E(\mathbf{x}, \mathbf{u}, \mathbf{u}_{(1)}, ...) = 0 \implies E(\hat{\mathbf{x}}, \hat{\mathbf{u}}, \hat{\mathbf{u}_{(1)}}, ...) = 0$

Example

$$\begin{aligned} & \star \begin{cases} \operatorname{div} \mathbf{u} = 0 \\ \mathbf{u}_t + (\nabla \mathbf{u})\mathbf{u} + \frac{1}{\rho}\nabla p - \nu\Delta \mathbf{u} + \beta g\theta \mathbf{e}_2 = 0 \\ \theta_t + \nabla \theta \cdot \mathbf{u} - \kappa\Delta\theta = 0 \end{cases} \\ & \star & \text{Symmetries: } (t, x, u) \longmapsto \\ & \bullet \quad (t + \epsilon, \mathbf{x}, \mathbf{u}) \\ & \bullet \quad (t, \mathbf{x} + \alpha(t), \mathbf{u} + \dot{\alpha}, p - \rho(\mathbf{x} + \alpha) \cdot \ddot{\alpha}, \theta) \\ & \bullet \quad (t, \mathbf{x}, \mathbf{u}, p + \zeta(t), \theta) \\ & \bullet \quad (t, \mathbf{x}, \mathbf{u}, p + \epsilon\beta g\mathbf{x} \cdot \mathbf{e}_2, \theta + \theta + \frac{\epsilon}{\rho}) \\ & \bullet \quad (t, \mathbf{Rx}, \mathbf{Ru}, p, \theta) \\ & \bullet \quad (\mathbf{e}^{2\epsilon} t, \mathbf{e}^{\epsilon} \mathbf{x}, \mathbf{e}^{-\epsilon} \mathbf{u}, \mathbf{e}^{-2\epsilon} p, \mathbf{e}^{-3\epsilon} \theta) \end{cases} \end{aligned}$$

 $\mathbb{G}=$ (4-dim Lie symmetry group) \lor (4 ∞ -dim symmetry groups)

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Importance of symmetry groups

- Traduce fundamental physical principles/properties (Galilean invariance, homogeneity, ...)
- Conservation laws through Noether's theorem
- Self-similar solutions
- Existence, stability, ... theorems, bifurcation
- Modeling (scaling laws, turbulence modeling, ...)

Invariant scheme and invariantization process

$$E\left(\mathbf{x},\mathbf{u},\mathbf{u}_{(1)},\ldots\right) = 0 \quad \begin{vmatrix} \mathbf{\underline{x}} = (\mathbf{x}^{1},\mathbf{x}^{2},\ldots), \ \mathbf{\underline{u}} = (\mathbf{u}^{1},\mathbf{u}^{2},\ldots), & \mathbf{u}^{i} \simeq \mathbf{u}(\mathbf{x}^{i}) \\ \operatorname{Schm}(\mathbf{\underline{x}},\mathbf{\underline{u}}) = 0 & \longleftarrow \begin{cases} \operatorname{Grid}(\mathbf{\underline{x}},\mathbf{\underline{u}}) = 0 \\ E_{h}(\mathbf{\underline{x}},\mathbf{\underline{u}}) = 0 \end{cases}$$

Invariant scheme and invariantization process

$$E\left(\mathbf{x}, \mathbf{u}, \mathbf{u}_{(1)}, \ldots\right) = 0 \quad \left| \begin{array}{c} \underline{\mathbf{x}} = (\mathbf{x}^{1}, \mathbf{x}^{2}, \ldots), \ \underline{\mathbf{u}} = (\mathbf{u}^{1}, \mathbf{u}^{2}, \ldots), \quad \mathbf{u}^{i} \simeq \mathbf{u}(\mathbf{x}^{i}) \\ \\ \mathrm{Schm}(\underline{\mathbf{x}}, \underline{\mathbf{u}}) = 0 \quad \underbrace{\mathrm{Schm}(\underline{\mathbf{x}}, \underline{\mathbf{u}}) = 0}_{E_{h}(\underline{\mathbf{x}}, \underline{\mathbf{u}}) = 0} \\ \\ \mathrm{Fin}(\underline{\mathbf{x}}, \mathbf{u}) \longmapsto (\widehat{\mathbf{x}}, \widehat{\mathbf{u}}) \\ \\ \underline{\mathbf{m}} \qquad \underline{\mathbf{m}} \qquad \underline{\mathbf{m}} \end{array} \right|$$

Invariant scheme and invariantization process $\underline{\textbf{x}}=(\textbf{x}^1,\textbf{x}^2,\dots),\;\underline{\textbf{u}}=(\textbf{u}^1,\textbf{u}^2,\dots),\qquad \textbf{u}^i\simeq \textbf{u}(\textbf{x}^i)$ $E\left(\mathbf{x},\mathbf{u},\mathbf{u}_{(1)},\ldots\right) = 0 \quad \text{Schm}(\underline{\mathbf{x}},\underline{\mathbf{u}}) = 0 \quad \textbf{\textbf{a}} \quad \begin{cases} \text{Grid}(\underline{\mathbf{x}},\underline{\mathbf{u}}) = 0 \\ E_h(\underline{\mathbf{x}},\underline{\mathbf{u}}) = 0 \end{cases}$ $T: (\mathbf{x}, \mathbf{u}) \longmapsto (\widehat{\mathbf{x}}, \widehat{\mathbf{u}}) \quad | \quad T_h: (\underline{\mathbf{x}}, \underline{\mathbf{u}}) \longmapsto (\underline{\widehat{\mathbf{x}}}, \underline{\widehat{\mathbf{u}}})$ m m m m Definition: scheme Schm is invariant if $\operatorname{Schm}(\mathbf{m}) = 0 \implies$ $\operatorname{Schm}(\widehat{\mathbf{m}}) = 0, \quad \forall T \in \mathbb{G}_F$ Sufficient condition $\operatorname{Schm}(\widehat{\mathbf{m}}) = \operatorname{Schm}(\mathbf{m})$ $\forall T \in \mathbb{G}_F$

Invariant scheme and invariantization process $\underline{\mathbf{x}} = (\mathbf{x}^1, \mathbf{x}^2, \dots), \ \underline{\mathbf{u}} = (\mathbf{u}^1, \mathbf{u}^2, \dots), \quad \mathbf{u}^i \simeq \mathbf{u}(\mathbf{x}^i)$ $\operatorname{Schm}(\underline{\mathbf{x}},\underline{\mathbf{u}}) = 0 \quad \longleftarrow \begin{cases} \operatorname{Grid}(\underline{\mathbf{x}},\underline{\mathbf{u}}) = 0\\ E_h(\underline{\mathbf{x}},\underline{\mathbf{u}}) = 0 \end{cases}$ $E\left(\mathbf{x},\mathbf{u},\mathbf{u}_{(1)},\ldots\right)=0$ $T: (\mathbf{x}, \mathbf{u}) \longmapsto (\widehat{\mathbf{x}}, \widehat{\mathbf{u}}) \mid T_h: (\underline{\mathbf{x}}, \underline{\mathbf{u}}) \longmapsto (\widehat{\mathbf{x}}, \widehat{\mathbf{u}})$ m m m m Definition: scheme Schm is invariant if $\operatorname{Schm}(\mathbf{m}) = 0 \implies$ $\operatorname{Schm}(\widehat{\mathbf{m}}) = 0, \quad \forall T \in \mathbb{G}_F$ Sufficient condition $\operatorname{Schm}(\widehat{\mathbf{m}}) = \operatorname{Schm}(\mathbf{m}) \qquad \forall T \in \mathbb{G}_F$ Invariatization process: Schm any scheme $\operatorname{Schm}(\underline{\mathbf{m}}) = \operatorname{Schm}(\tau[\underline{\mathbf{m}}] \cdot \underline{\mathbf{m}})$ is an invariant scheme (Right) Mobile frame: $\tau : \mathbf{m} \in M \mapsto \tau[\mathbf{m}] \in \mathbb{G}$ $\tau[T(\mathbf{m})] = \tau[\mathbf{m}]T^{-1}$ $\forall T \in \mathbb{G}$

Application

- Burgers equation: $\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} \nu \frac{\partial^2 u}{\partial x^2} = 0$
- 5-dim Lie symmetry group
 - Space translation:
 - Time translation:
 - Projection:
 - Scale transformation:
 - Galilean boost:

FTCS, Regular grid,

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} + u_i^n \left[\frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} \right] - \nu \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} = 0$$

Invariantized FTCS, Regular grid,

$$O(\Delta t, t)$$

$$\frac{u_{i}^{n+1}(1-\epsilon_{3}\Delta t)-u_{i}^{n}}{\Delta t}(1-\epsilon_{3}\Delta t)+\left[u_{i}^{n}+\epsilon_{5}\right]\left[\frac{u_{i+1}^{n}-u_{i-1}^{n}}{2\Delta x}+\epsilon_{3}\right]-\nu\frac{u_{i+1}^{n}-2u_{i}^{n}+u_{i-1}^{n}}{\Delta x^{2}}=0$$

$$\epsilon_3 = \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x}, \quad \epsilon_5 = fu_{i+1}^n + eu_i^n + fu_{j-1}^n, \quad e+2f = 1$$

$$(t + \epsilon_1, x, u) (t, x + \epsilon_2, u) (\frac{t}{1 - \epsilon_3 t}, \frac{x}{1 - \epsilon_3 t} + \epsilon_3, u(1 - \epsilon_3 t) + \epsilon_3 x) (e^{2\epsilon_4} t, e^{\epsilon_4} x, e^{-\epsilon_4} u) (t, x + \epsilon_5 t, u + \epsilon_5)$$

$$O(\Delta t, \Delta x^2)$$

Numerical results

Pseudo-choc :
$$u(t,x) = \frac{\sinh\left(\frac{x}{2\nu}\right)}{\cosh\left(\frac{x}{2\nu}\right) + \exp\left(\frac{-t}{4\nu}\right)}$$



Left: $\nu = 8 \cdot 10^{-3}$. Right: $\nu = 7.5 \cdot 10^{-4}$

Self-similar solution under projection

Numerical results



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- Invariant integrator: conclusion
 - ★ Compatibility with fundamental invariance properties
 - ★ Compatibility with self-similar solutions
 - ★ May have sensibly higher numerical cost But more interesting for coarse time/space grids
 - $\star~$ Should not destroy conservation laws and symmetry based models
 - ★ To be done for Navier-Stokes equations

Problems for which other properties are more important ?

★ Many Navier-Stokes solvers use : curl grad = 0, div curl = 0

Eg: vorticity-stream function formulation

Not numerically verified \Longrightarrow spurious mass, portance, circulation, ...

★ In exterior calculus: $d^2 = 0$ $d : \Lambda^k \longrightarrow \Lambda^{k+1}$: exterior derivative operator

acting on differential forms

Discrete Exterior Calculus: Discrete version of Exterior Calculus theory



Discrete Exterior Calculus (DEC)

Exterior and differential forms

Exterior k-form = skew-symmetric k-linear form

Differential k-form $\omega \in \Lambda^k(M)$: Smooth field of exterior k-forms $\omega_{|_X} : T_{\mathbf{x}}M \times \ldots \times T_{\mathbf{x}}M \longrightarrow \mathbb{R}$

Locally: $\omega = \omega_{i_1 \dots i_k}(\mathbf{x}) dx^{i_1} \wedge \dots \wedge dx^{i_k}$

• Often derivated:
$$\Lambda^0 \xrightarrow{d} \Lambda^1 \xrightarrow{d} \Lambda^2 \xrightarrow{d} \dots$$
 with $d^2 = 0$
 $Locally: d\omega = \frac{\partial \omega_{i_1 \dots i_k}}{\partial x^j} dx^j \wedge dx^{i_1} \wedge \dots \wedge dx^{i_k}$
• $d: \Lambda^0 \longrightarrow \Lambda^1 \longrightarrow grad: \mathcal{F}(R^3) \longrightarrow \mathfrak{X}(R^3)$
• $d: \Lambda^2 \longrightarrow \Lambda^3 \longrightarrow div : \mathfrak{X}(R^3) \longrightarrow \mathcal{F}(R^3)$
• $d^2 = 0 \longrightarrow rot grad = 0, div rot = 0$

Sometimes integrated: $\omega : \sigma \longmapsto \int_{\sigma} \omega$

 $M \text{ orientable manifold, } \omega \in \Lambda^k(M), \quad \sigma \text{ k-dim submanifold of } M$ Stokes: $\int_{\sigma} d\omega = \int_{\partial \sigma} \iota_{\partial \sigma}^* \omega$

Discretization



More formally : combinatorial geometry

★ k-simplex
$$[\mathbf{v}_0\mathbf{v}_1\dots\mathbf{v}_k] = \left\{\sum_{i=0}^k \lambda_i\mathbf{v}_i, \ \lambda_i \ge 0, \sum_{i=1}^k \lambda_i = 1\right\} \in K_k$$

★ Simplicial complex: Collection $K = \bigcup_{k=0}^{n} K_k$ of simplices such that

- $\sigma \in K$ and τ face of $\sigma \implies \tau \in K$
- + regularity conditions
- ★ Orientation

Mesh

Chain = Element of
$$\Lambda_k(K)$$
 $|K_k|$ -dim array
 $\star \quad \Lambda_k(K) = \operatorname{span}_{\mathbb{Z}} K_k = \left\{ \sum_{\sigma \in K_k} z_\sigma \sigma, \ z_\sigma \in \mathbb{Z} \right\}$
 $\partial \stackrel{(K_k)}{\longrightarrow} = \stackrel{(K_k)}{\longrightarrow}$

★ Boundary operator

Extends by linearity into $\partial : \Lambda_k(K) \longrightarrow \Lambda_{k-1}(K)$

Discrete k-form = k-cochain = Element of $\Lambda^{k}(K)$ $|\kappa_{k}|$ -dim array $\star \quad \Lambda^{k}(K) = \mathbb{R}$ -dual of $\Lambda_{k}(K) \simeq \left\{ \sum_{\sigma \in K_{k}} \omega_{\sigma} \sigma, \ \omega_{\sigma} \in \mathbb{R} \right\}$ $\star \quad \text{Discrete } d = \partial^{\top} : \Lambda_{k}(K) \longrightarrow \Lambda_{k+1}(K)$ $(|\kappa_{k+1}| \times |\kappa_{k}|)$ -dim array

Hodge ***** operator

M: *n*-dim manifold M with metric g and volume form vol

Continuous Hodge: isomorphism $\star : \Lambda^k(M) \longrightarrow \Lambda^{n-k}(M)$ such that $\theta \land \star \omega = g(\theta, \omega)$ vol• Complement to vol: $\omega \land \star \omega =$ volif $g(\omega, \omega) = 1$ Orthogonality: $g(\star \omega, \omega) = 0$

In ℝ² with Euclidean metric and vol = dx ∧ dy *1 = dx ∧ dy, *dx = dy, *dy = -dx, *dx ∧ dy = 1
In ℝ³ with Euclidean metric and vol = dx ∧ dy ∧ dz

$$\star 1 = \mathrm{d} x \wedge \mathrm{d} y \wedge \mathrm{d} z, \qquad \star \mathrm{d} x = \mathrm{d} y \wedge \mathrm{d} z, \qquad \star (\mathrm{d} x \wedge \mathrm{d} y) = \mathrm{d} z, \qquad \dots$$

• dim
$$\Lambda^k(M) = \binom{n}{k} = \binom{n}{n-k} = \dim \Lambda^{n-k}(M)$$

Usefull to formulate constitutive laws

Dual mesh

Discrete Hodge: isomorphism ?

 $\star: \Lambda^k(K) \longrightarrow \Lambda^{n-k}(K)$ Generally impossible

$$\dim \Lambda^k(K) = |K_k| \neq |K_{n-k}| = \dim \Lambda^{n-k}(K)$$

Eg when n = 2: nb vertices \neq nb triangles



Dual mesh

Discrete Hodge: isomorphism ?

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Eg when n = 2: nb vertices \neq nb triangles

Discrete Hodge: isomorphism

$$\star: \Lambda^k(K) \longrightarrow \Lambda^{n-k}(*K)$$
 Possible

► Dual mesh
$$*K = \bigcup_{k=0}^{n} (*K)_k$$

★ Bijection $*: K_k \longrightarrow (*K)_{n-k}$
★ Orientation on $K \longrightarrow$ Orientation on $*K$
★ Dual cochain: element of $\Lambda^k(*K)$
★ ∂ on $K \longrightarrow$ ∂ on $*K \longrightarrow$ d on $*K$



Circumcentric dual

• dim
$$\Lambda^k(K) = |K_k| = |(*K)_{n-k}| = \dim \Lambda^{n-k}(*K)$$

Discrete Hodge operator

- How to define $\star : \Lambda^k(K) \longmapsto \Lambda^{n-k}(*K)$?
- Continuous case : If ω is locally constant and $\sigma \perp *\sigma$

(circumcentric dual)

$$\frac{1}{|*\sigma|}\int_{*\sigma}\star\omega=\frac{1}{|\sigma|}\int_{\sigma}\omega, \qquad \qquad |\sigma|=\begin{cases} k\text{-volume de }\sigma, & \dim\sigma\geq 1\\ 1 & \dim\sigma=0 \end{cases}$$

 Circoncentric Hodge

 $\frac{\langle \star \omega, \ast \sigma \rangle}{|\ast \sigma|} = \frac{\langle \omega, \sigma \rangle}{|\sigma|}$

 Diagonal matrix $H_k = \text{diag}\left(\frac{|\ast \sigma|}{|\sigma|}, \quad \sigma \in K_k\right)$

Navier-Stokes + passive scalar (polluant)

Vector/tensor formulationExterior calculus formulation $(\omega = u^b)$ $\frac{\partial \mathbf{u}}{\partial t} + \operatorname{div}(\mathbf{u} \otimes \mathbf{u}) + \frac{1}{\rho} \operatorname{grad} p - \nu \Delta \mathbf{u} = 0$ $\frac{\partial \omega}{\partial t} + u _ \mathrm{d}\omega + \frac{1}{\rho} \mathrm{d}\left(p + \frac{1}{2}\rho||\mathbf{u}||^2\right) - \nu \delta \mathrm{d}\omega = 0$ $\frac{\partial \theta}{\partial t} + \operatorname{div}(\mathbf{u}\theta) - \kappa \Delta \theta = 0$ $\frac{\partial \omega}{\partial t} + \omega \mathrm{d}\omega + \frac{1}{\rho} \mathrm{d}\left(p + \frac{1}{2}\rho||\mathbf{u}||^2\right) - \nu \delta \mathrm{d}\omega = 0$ $\frac{\partial \theta}{\partial t} + \operatorname{div}(\mathbf{u}\theta) - \kappa \Delta \theta = 0$ $\frac{\partial \theta}{\partial t} + \delta(\omega \wedge \theta) - \kappa \delta \mathrm{d}\theta = 0$

 $\delta=\pm\star\,\mathrm{d}\star$

Resolution: Stream function $\omega = - \star d\psi$

Consequence: div $\mathbf{u} = \mathbf{0}$ at machine precision







Concentration of polluant at different times

Necessity of an alternative discrete Hodge Circumcentric Hodge needs a "well-centered" primal mesh







- Change simplex centers
 - ★ barycenter, incenter, ...
 - ★ error minimisation
 - ★ physical consideration



"Analytical" discrete Hodge

Any dual mesh (circumcenter, barycenter, incenter, ...)

• Exact if ω locally constant

$$H_{1} = \begin{pmatrix} \frac{|*e_{1}|}{|e_{1}|} & 0 & 0\\ 0 & \frac{|*e_{2}|}{|e_{2}|} & 0\\ 0 & 0 & \frac{|*e_{2}|}{|e_{2}|} \end{pmatrix} \begin{pmatrix} \sin\theta_{1} & a_{1}^{2}\cos\theta_{1} & a_{1}^{3}\cos\theta_{1} \\ a_{1}^{2}\cos\theta_{2} & \sin\theta_{2} & a_{2}^{3}\cos\theta_{2} \\ a_{3}^{1}\cos\theta_{3} & a_{3}^{2}\cos\theta_{3} & \sin\theta_{3} \end{pmatrix}$$

• $\theta_i = (\widehat{\vec{e}_i, \vec{*e}_i}), \quad -R_{\pi/2}\vec{e}_1 = a_1^2\vec{e}_2 + a_1^3\vec{e}_3, \ldots$

[Ayoub, Hamdouni, Razafindralandy. AMC 2021]

Example in an unitary triangle



$$H_1^{\text{barycenter}} = \frac{1}{6} \begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad H_1^{\text{incenter}} = \frac{1}{4 + 2\sqrt{2}} \begin{bmatrix} 2 & \sqrt{2} & 0 \\ \sqrt{2} & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

- Invertible
- Assembling
- Elementwise inversion



Poisson Equation

 $\blacktriangleright \quad \Delta \omega = \overline{f}$

Exterior calculus formulation: $\star d \star d \omega = f$

Well-centered mesh

- ★ Circumcentric dual
- ★ Barycentric dual



Acute mesh

- ★ Barycentric dual
- ★ Incentric dual



 $\Delta x_{mean} =$ mean edge length

Poisson equation



 $\omega_{exact} = \sin(\pi x) \sinh(\pi y)$

Navier-Stokes: Taylor-Green Vortex

 $u = -\cos x \sin y e_x + \sin x \cos y e_y$



Anisothermal traveling wave

$$\begin{split} \xi &= \mathsf{a}\mathsf{x} + \mathsf{b}\mathsf{y} + \mathsf{c}\mathsf{t}, \quad \mathbf{u} = (\alpha_1 \, \mathsf{e}^{\lambda\xi/\nu} + \alpha_2 \, \mathsf{e}^{\lambda\xi/\tau}) \, \mathsf{e}_\mathsf{x} + \alpha_3 \, \mathsf{e}_\mathsf{y} \\ p &= \alpha_p \, \mathsf{e}^{\lambda\xi/\tau}, \qquad \theta = \alpha_\theta \, \mathsf{e}^{\lambda\xi/\tau} \end{split}$$

The α . are non-independent constants



Dual mesh	Stream function	Velocity	Temperature	
Barycentric	$2.651 \cdot 10^{-5}$	$7.270 \cdot 10^{-5}$	$5.529 \cdot 10^{-3}$	
Incentric	$8.875 \cdot 10^{-5}$	$2.132 \cdot 10^{-4}$	$5.589 \cdot 10^{-3}$	
NA Lut				

Mean relative error

In both cases, div u = 0 at machine precision











(a) $\Delta x_{mean} = 0.2682$

682 (b) $\Delta x_{mean} = 0.1265$ (c) $\Delta x_{mean} = 0.0650$



(d) $\Delta x_{mean} = 0.0328$ Ex: 50% of non-Delaunay triangles











(a) $\Delta x_{mean} = 0.2682$ (b) $\Delta x_{mean} = 0.1265$ (c) $\Delta x_{mean} = 0.0650$



θ
1.5159
1.2154
0.8660
1

Convergence rate

(d) $\Delta x_{mean} = 0.0328$ Ex: 50% of non-Delaunay triangles

On a surface

Initial flow: $\psi(t=0) = y + 0.1z$,

40% of well-centered triangles



Streamlines for t from 0 to 11



Conclusion

Done

- ★ "Velocity"-pressure formulation + Prediction-correction scheme Lid driven cavity (Ghia), Re=100, Re=1000
- ★ Neumann boundary condition
- ★ 3D with Whitney Hodge
- Advantages
 - \star d² = 0
 - ★ Coordinate independent
 - ★ Exterior calculus formulation brings clarity in some problems
 - ★ Conservation laws : Circulation preservation for non-viscous fluid Needs carefully designed time integrator
- To do
 - **★** Further exploitatiion of $d^2 = 0$
 - Complex geometry
 - ★ Space-time DEC
 - ★ Invariantized space-time DEC ?