

动边界不可压流体的数学理论 及时空一致四阶精度有限体积方法

第五届"设计+运维"国产工业软件研讨会 暨2023年天洑软件用户大会



动边界不可压流体



核心困难

- 多个流相耦合
- 动边界几何上的大变形;
- 流相潜在的拓扑变化;
- 物理量在界面处不连续;











现有数值方法



基于连续介质的数学模拟+界面追踪算法

- Immersed Boundary Method; Immersed Interface Method
- Level Set Method; Volume-of-fluid method
- Arbitrary Lagrangian-Eulerian Method

粒子方法

- Lattice Boltzmann
- Smoothed Particle Hydrodynamics
- •••

共同核心理念: **将几何和拓扑问题转化成数值偏微分方程问题予以回避** $\frac{\partial f}{\partial t} + \nabla \cdot (f\mathbf{u}) = 0$



在等距变换的流场下无法保持流相的几何特征

 \star rotation





在同胚映射的流场下无法保持流相的拓扑结构

★ vortex shear



现有方法的局限性:快速得到整体拓扑信息?



难以得到流相的拓扑信息:

- 连通分量个数
- 连通区域中空洞的个数
- 亏格
- 贝蒂数
- 欧拉示性数





如何度量计算精度和计算效率



■ 求解问题的一般手段:物理现象→数学模型→数值模拟。求解问题的误差可以表示为

 $\boldsymbol{E}_{\text{total}} = \boldsymbol{E}_{\text{model}} + \boldsymbol{E}_{\text{solve}}$

其中 E_{total} 是总体误差, E_{model} 是模型误差, E_{solve} 是计算误差。

■ 记 U^n 为数学模型在 t_n 时刻的真实解, \widehat{U}_h^n 是通过某数值方法得到的数值解,如果

 $\forall T > 0, \lim_{k \to 0, h \to 0, k \to 0} \|\boldsymbol{E}_{h}^{N}\| = 0,$

这里 $E_h^N = U^N - \widehat{U_h^N}$, k, h 分别是时间步长和空间步长。我们称该数值方法是收敛的。

■ 对于一个数值方法,如果存在一个常数C,使得对于充分小的k,h,

 $\|\boldsymbol{E}_{\boldsymbol{h}}^{N}\| \leq C(h^{p} + k^{q}),$

则称该数值方法在空间上是 p 阶收敛, 在时间上是 q 阶收敛的。

■ 阶数越高,收敛越快:计算精度和计算效率在一定程度上等价。

■ 时空一致四阶算法的必要性: 空间上二十阶收敛 + 时间上一阶收敛 = 一阶收敛。

とぶ 先活

■ 时空一致四阶算法的特殊性:对三维Navier-Stokes方程来说收入和产出是成正比的。



界面的线性二阶表示:

- 界面表示和追踪效率低
- 曲率估算误差大

流速场最高一阶或二阶精度:

一些物理过程决定于流速的高阶导数项

- 无滑移边界条件: 切向流速的法向梯度 $\frac{\partial u_{\tau}}{\partial n}$
- 边界层分离:转捩点的位置满足 $\frac{\partial^2 u_{\tau}}{\partial n^2} = 0$

高精度 + 保结构 →	真实反映物理实际
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10^{-4}	10^{-6}	10^{-8}	10^{-10}
42e-01	1.42e-02	1.42e-03	1.42e-04

第一行: 界面追踪误差 第二行: 曲率估算的最小误差 <u>张庆海 2017 SIAM J. Numer. Anal.</u>



用几何和拓扑的工具解决几何和拓扑的问题!

- Yin Space: 连续介质几何位置和拓扑结构的数学模型及布尔代数 <u>张庆海 and Li 2020 Math. Comput.</u>
- MARS: 界面追踪问题的理论分析框架 <u>张庆海 2013 SIAM Review; 张庆海 2013, 2016 SIAM J. Numer. Anal.; 2019 SIAM J. Sci. Comput.</u>
- cubic MARS & HFES: 四阶及以上精度的界面追踪和曲率估计方法 <u>张庆海 et. al. 2014,2018 SIAM J. Sci. Comput.; 张庆海 2017 SIAM J. Numer. Anal.</u>
- GePUP: 时空一致四阶精度求解Navier-Stokes方程的有限体积法(并行+自适应) <u>张庆海 et. al. 2012 SIAM J. Sci. Comput.; 张庆海 2016 J. Sci. Comput.</u>
- 处理不规则边界的人工智能算法 <u>张庆海 et. al. 2023 under review</u>
- 耦合以上模块发展动边界不可压流体的高保真算法和软件 <u>张庆海 et. al. 2017- in progress</u>

基于锐利界面的数学模型





连续介质流相之间由锐利界面隔开

- 如何对单一流相实现高精度算法?
- 如何表示和追踪动边界?
- 如何将界面的本构关系反映到算法中?
- 如何耦合各个模块以最大化灵活性?

▶ 为动边界流体量身订制一整套数学理论

▶ 为动边界流体的数值模拟发展<u>时空一致四阶精度</u>算法

连续介质的数学模型: 殷集和殷空间



(\mathbb{S},\mathbb{Y}) : a topological space where

 $\mathbb{S}:$ regular semianalytic sets with bounded boundaries.

$\mathbb{Y}_{\mathbb{C}}$ regular open semianalytic sets with bounded boundaries.

Physical requirement	Physical requirements		
continuum hypothe	continuum hypothesis		
piecewise smooth bou	semianalytic sets		
computable	bounded boundary		
Topological info	mology on C-W Compley	Xes	
		hology on e tt complex	~~~
# of connected components	the zeroth Betti number		
# of holes	rst and second Betti nur	nbers	

Computational homology for Betti numbers:

- an overkill for simulating multiphase flows,
- In high complexities of Betti-number computation.





★ 拓扑结构可以任意复杂

★0(1)时间返回拓扑示性数







★ 拓扑结构可以任意复杂

★ 适用于所有退化情况

★ 接近最优复杂度

★ 可直接推广到三维空间

三维连续介质的高效表示和布尔代数



定理(张庆海 and Liang 2023)

三维殷集的边界同胚于二维紧流形在一维胞腔复形上的商空间





标量守恒律的捐献区间理论



- 对动力系统中拉格朗日粒子按照其曲线穿透次数进行分类
- 对标量守恒律 $\frac{\partial f}{\partial t} + \nabla \cdot (f\mathbf{u}) = 0$ 证明了以下通量解析表达式:

$$\int_{t_0}^{t_0+\kappa}\int_{\widetilde{LN}}f\,\mathbf{u}\cdot\mathbf{n}_{\widetilde{LN}}\,\mathrm{d}s\,\mathrm{d}t=\sum_{n\in\mathbb{Z}}n\int_{\mathcal{D}_{\widetilde{LN}}^n(t_0,k)}f(\mathbf{x},t_0)\mathrm{d}\mathbf{x}=\oint_{\gamma_{\widetilde{LN}}}F(x,y,t_0)\mathrm{d}y,$$







method.

Finally, Zhang [27] has presented a rigorous mathematical analysis of the VOF-advection through the prism of differential geometry and Boolean algebra. It demonstrates that the *edgewise* approach of the problem (based on the flux balance of the volume), is theoretically equivalent to a *cellwise* approach, where the liquid volume of the entire cell is retrieved by

"Zhang has presented a rigorous mathematical analysis of VOF-advection through the prism of differential geometry and Boolean algebra."

"用微分几何和布尔代数为VOF 方法提供了严格的数学分析"



★ 时空一致四阶精度
 ★ 分离流相、界面、和曲率估计的三个尺度
 ★ 0(1)复杂度返回拓扑示性数
 ★ 保持几何特征和拓扑结构

















Methods	32 ²	rate	64 ²	rate	128 ²		
cubic MARS $(h_L = 0.2h)$	7.22e-07	4.97	2.30e-08	5.00	7.17e-10		
cubic MARS $(h_L = 0.5h^{\frac{3}{2}})$	3.67e-09	8.01	1.43e-11	6.91	1.19e-13		
cubic MARS $(h_L = 2h^2)$	9.85e-11	8.50	2.72e-13	10.26	2.22e-16		
Rider/Kothe/Puckett	4.78e-02	2.78	6.96e-03	2.27	1.44e-03		
Stream/Youngs	3.61e-02	1.85	1.00e-02	2.22	2.16e-03		
Improved PLIC-VOF	5.78e-03	1.71	1.77e-03	2.42	3.30e-04		
AMR-MOF (2009)	2.33e-02	2.89	3.15e-03	2.64	5.04e-04		
Hybrid markers	2.52e-03	2.96	3.23e-04	2.99	4.06e-05		
LS-WENO-5 (2008)	—	_	_	_	2.32e-03		
RKDG-CLS-4 (2017)	_	_	3.43e-03	2.3	7.06e-04		
[Z and Fogelson 2014, SIAM J. Sci. Comput] [Z and Fogelson 2016, SIAM J. Numer. Anal]							
Z 2017, SIAM J. Numer. Anal] Z 2018, SIAM J. Sci. Comput]							

Curvature Estimation results based on the vortex-shear test.

Test	$h = \frac{1}{32}$	rate	$h = \frac{1}{64}$
8th-order MARS+HFES [Z 2017 SINUM]	4.76e-08	7.78	2.17e-10
2nd-order VOF+HF method [Sussman 2003 JCP]	3.31e-01	2.23	7.06e-02



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A-SLEIPNNIR: A multiscale, anisotropic adaptive, particle level set framework for moving interfaces. Transport equation applications

Juan Luis Prieto *, Jaime Carpio

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西班牙马德里理工大学Prieto教授 (J. Comput. Phys. 2019)

DT scheme. For Rudman's version of the test, A-SLEIPNNIR trails, in terms of the e_{l1}^* of Eq. (14) just behind the remarkable iPAM method by Zhang and Fogelson, for both the linear version [28], and the most recent cubic iPAM presented in the MARS framework [29].

Table 3 Comparison of A-SLEIPNNIR with published results: circular droplet in periodic ($T_p = 8$), single vortex flow. NE and NC are the number of elements and nodes, respectively, at time t = 4 (maximum deformation). All data extracted from the cited references.

Method [Ref.]	h_{\min}^{-1}	$h_{\rm max}^{-1}$	С	Np	NE	NC	<i>e</i> _{<i>L</i>¹}	$\Delta A/A_0(\%)$
EMFPA-V ^{cor} [67]	≈128	≈128	0.500		15886	8112	$1.02 imes 10^{-2}$	Machine
Rider-Kothe (Puckett) [72]	128	128	1.000		16384	16384	1.44×10^{-3}	N/A
HPLS HJ-WENO [23]	128	128	0.500	\approx 80000	16384	16384	1.40×10^{-3}	$7.90 imes10^{-1}$
CCU [27]	128	128	1.000	N/A	16384	16384	1.00×10^{-3}	Machine
SLPLS [24]	128	128	4.900	\approx 20000	16384	16384	$9.73 imes 10^{-4}$	$7.30 imes10^{-1}$
NBLR-LS WENO [31]	128	128	1.000		>16384	>16384	7.00×10^{-4}	$6.80 imes 10^{-1}$
ACLSVOF-A [71]	\approx 128	10	N/A		2246	2246	5.09×10^{-4}	$1.30 imes 10^{-4}$
AMR-MOF [32]	128	32	4.000		>1672	>1672	5.04×10^{-4}	7.09×10^{-13}
Mark-C-VOF [75]	128	128	1.000	5813	16384	16384	4.06×10^{-5}	$7.38 imes 10^{-3}$
A-SLEIPNNIR	128	2	1.280	50000	2780	5573	2.83×10^{-5}	$1.40 imes 10^{-5}$
iPAM linear h ² [28]	128	128	1.000	N/A	16384	16384	1.17×10^{-8}	Machine
iPAM cubic 5h ² [29]	128	128	1.000	N/A	16384	16384	7.92×10^{-10}	Machine

in the latter case, come at the price of a notably higher computational cost. And then, there is the iPAM method by Zhang and Fogelson, which, as it happened in the solid-body rotation test, performs at another level of accuracy due to its fourthorder convergence with uniform spatial refinement. Besides, the recent unsplit VOF method (CCU) proposed by Comminal "the **remarkable** iPAM

method by Zhang"

"And then, there is the iPAM method by Zhang and Fogelson, which, ..., performs at another level of

accuracy due to its fourthorder convergence ... "

"张的四阶方法在另一个精度 水平上"



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Table 3

iPAM cubic 5h² [29]

128

128

1.000

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16384

16384

 $7.92 imes 10^{-10}$

Machine

N/A





✓ 现代数学物理的核心:不可压 Navier-Stokes 方程

- D. Hilbert, 1900@ IMU: 23 个数学问题;
- S. Smale, 1997@ IMU: 18 个 21 世纪最重要的数学问题;
- Clay 研究所, 2000: 七个千禧年大奖难题。

✓ 关于 Navier-Stokes 方程的千禧年问题:

- 解的存在性以及光滑性: ℝ³ 空间以及ℝ³/ℤ³ (3 torus);
- 有限时间内爆破的反例: ℝ³空间以及ℝ³/ℤ³ (3 torus)。



- 泊松方程、对流扩散方程的并行自适应有限体积方法 <u>张庆海 2011 Comput. Methods Appl. Mech. Engrg.;</u> <u>张庆海 et. al. 2012 SIAM J. Sci. Comput.;</u> <u>张庆海 2013 Comput. Methods Appl. Mech. Engrg.</u>
- 周期边界条件Navier-Stokes方程的自适应四阶近似投影方法 <u>张庆海 2014 Appl. Numer. Math.</u>
- ★ 无滑移边界条件Navier-Stokes方程的四阶广义投影方法GePUP <u>张庆海 2016 J. Sci. Comput.</u>
- ★ Navier-Stokes方程+对流扩散方程组的四阶有限体积方法 <u>张庆海 2023 under review</u>





$$\frac{\partial w}{\partial t} = g - u \cdot \nabla u - \nabla q + \nu \Delta w \text{ in } \Omega, \quad (29a)$$

$$w = 0 \text{ on } \partial \Omega, \quad (29b)$$

$$u = \mathscr{P}w \text{ in } \Omega, \quad (29c)$$

$$u \cdot n = 0 \text{ on } \partial \Omega, \quad (29d)$$

$$\Delta q = \nabla \cdot (g - u \cdot \nabla u) \text{ in } \Omega, \quad (29e)$$

$$n \cdot \nabla q = n \cdot (g + \nu \Delta u - \nu \nabla \nabla \cdot u) \text{ on } \partial \Omega. \quad (29f)$$

- The single evolution variable in (29) is w, with u a function of w and q a function of u.
- $\nabla \cdot w$ decays so long as we impose $\nabla \cdot w = 0$ on $\partial \Omega$:

$$\frac{\partial (\nabla \cdot \mathbf{w})}{\partial t} = \nu \Delta (\nabla \cdot \mathbf{w}). \tag{30}$$







- Spatial boundary conditions are independent of time integration;
- The space of solvers is spanned by orthogonal policies such as spatial discretization and time integration;



Classical finite-volume discretization on rectangular cells,

$$\langle \phi \rangle_{i} := \frac{1}{h^{\mathsf{D}}} \int_{\mathcal{C}_{i}} \phi(\mathbf{x}) \, \mathrm{d}\mathbf{x},$$
 (31)

with discrete operators acting on cell averages, e.g.

$$\mathsf{L} \langle \phi \rangle_{\mathsf{i}} := \frac{1}{12h^2} \sum_{d} \left(-\langle \phi \rangle_{\mathsf{i}+2\boldsymbol{e}^d} + 16 \langle \phi \rangle_{\mathsf{i}+\boldsymbol{e}^d} - 30 \langle \phi \rangle_{\mathsf{i}} + 16 \langle \phi \rangle_{\mathsf{i}-\boldsymbol{e}^d} - \langle \phi \rangle_{\mathsf{i}-2\boldsymbol{e}^d} \right),$$

$$\mathsf{P} := \mathsf{I} - \mathsf{GL}^{-1}\mathsf{D},$$

$$\mathsf{P}^2 \neq \mathsf{P}, \qquad \mathsf{P} \langle \mathsf{u} \rangle_{\mathsf{i}} - \frac{1}{h^{\mathsf{D}}} \int_{\mathcal{C}_{\mathsf{i}}} \mathscr{P} \mathsf{u} = O(h^4), \qquad \rho(\mathsf{P}) = 1.$$

$$(33)$$



The ODE system after spatial discretization of GePUP:

$$\frac{\mathrm{d} \langle \mathsf{w} \rangle}{\mathrm{d}t} = \langle \mathsf{g} \rangle - \mathsf{D} \langle \mathsf{u}\mathsf{u} \rangle - \mathsf{G} \langle q \rangle + \nu \mathsf{L} \langle \mathsf{w} \rangle, \qquad (34a)$$

$$\langle \mathsf{u} \rangle = \mathsf{P} \langle \mathsf{w} \rangle, \qquad (34b)$$

$$\langle q \rangle = \mathsf{L}^{-1} \mathsf{D} (\langle \mathsf{g} \rangle - \mathsf{D} \langle \mathsf{u}\mathsf{u} \rangle), \qquad (34c)$$

- 不存在任何非物理的边界条件
- 空间离散与时间积分完全解耦

自适应网格+并行计算







求足創析





The initial condition is a pure rotational velocity field projected by P.

h	$\frac{1}{256} - \frac{1}{512}$	Rate	$\frac{1}{512} - \frac{1}{1024}$	Rate	$\frac{1}{1024} - \frac{1}{2048}$
$-$ u L_{∞}	9.61e-04	3.66	7.60e-05	3.85	5.26e-06
u <i>L</i> ₁	3.92e-05	3.78	2.85e-06	3.90	1.91e-07
u <i>L</i> ₂	7.44e-05	3.76	5.51e-06	3.88	3.73e-07
$p L_{\infty}$	7.01e-06	3.78	5.09e-07	3.90	3.40e-08
<i>p L</i> ₁	9.00e-07	3.81	6.41e-08	3.90	4.29e-09
р L ₂	1.41e-06	3.80	1.01e-07	3.90	6.77e-09
$\overline{\nabla imes u \ L_\infty}$	2.20e-01	2.75	3.26e-02	3.12	3.74e-03
$\nabla imes$ u L_1	3.90e-03	3.60	3.22e-04	3.85	2.24e-05
$\nabla imes$ u L_2	1.15e-02	3.29	1.17e-03	3.71	8.97e-05

张庆海, 2016, J. Sci. Comput.

即使只要求涡量计算结果有两位有效数字,GePUP方法也能把美国科学院院士 Colella的经典二阶投影方法的计算效率或计算精度提高上万倍!

不规则边界处理算法:人工智能+数值逼近





浙江大学

将计算域嵌在一个矩形区域里,以规则网格划分控制体。

- 1. 静止欧拉网格算流场;运动拉格朗日网格追踪界面;
- 2. 按照控制体和不规则边界的相对位置对控制体分类;
- 3. 规则控制体用经典差分模板离散,不规则控制体用不规则模板离散;
- 4. 求解离散后的方程组。





如何为不规则节点选择一组附近的节点使得高阶完全多项式的拟合存在且唯一?





不规则边界处理算法:人工智能搜索算法



如何找到从 Arad 到 Bucharest 的最短路径?

- 1. 生成解空间
- 2. 在解空间上进行搜索





不规则边界处理算法:人工智能算法的新问题

み経

梁阳





不规则边界处理算法:人工智能+抽象代数



Theorem (Z. and Li)

Suppose $\Lambda_d \subset \mathbb{Z}_n$ for $1 \leq d \leq D$, and A is an arbitrary D-permutation. Define \mathcal{B} to be the collection of D-permutations that agree with A on $\{\Lambda_d\}_1^D$. Then we have

我们找到了最优的 解空间生成方法。 $AW = \bigcap_{B \in \mathcal{B}} B\mathcal{P}$

as subsets of \mathbb{Z}_n^D , where \mathcal{P} is the principal lattice, and

$$W = W(\{\Lambda_d\}_1^D) = \left\{ p \in \mathbb{Z}_n^D : \prod_{d=1}^D W^+(p_d, \Lambda_d) \subset \mathcal{P} \right\}; \quad (81)$$
$$W^+(c, \Lambda) := \left\{ \begin{aligned} \{c\} & c \in \Lambda, \\ \mathbb{Z}_n \setminus \Lambda & c \notin \Lambda. \end{aligned} \right. \tag{82}$$



不规则边界处理算法:适定节点生成结果





(a) A convex surface









(c) The corner of a box

在静止不规则边界上的时空一致四阶精度方法





user: zyk Tue May 3 19:40:19 2022

含刚性动边界的时空一致四阶精度方法



t = 0, 0.1, 0.25, 0.50, 0.75, 1.0



Re=100	$\frac{1}{20} - \frac{1}{40}$	rate	$\frac{1}{40} - \frac{1}{80}$	rate	$\frac{1}{80} - \frac{1}{160}$
u, L^{∞}	1.66e-01	2.62	2.72e-02	3.59	2.26e-03
u, <i>L</i> 1	6.69e-03	3.11	7.74e-04	3.26	8.06e-05
u, <i>L</i> ²	1.38e-02	3.07	1.65e-03	3.47	1.49e-04

含刚性动边界的时空一致四阶精度方法







动边界不可压流体的时空一致四阶精度有限体积法





1

正在进行的工作:

▶ 将三维界面追踪方法与不可压流体的四阶投影方法耦合

▶ 针对具体问题发展特定的工业软件,如热管理、流固耦合等

求走創祈





请提宝贵意见!