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博士学位论文

可压缩流动中间断问题的高分辨率数值求解方法及应用

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A Study of High-Resolution Algorithms for Discontinuous Problems in Complex Compressible Flows and Their Applications

By

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插图

第一章　双信息保存方法（Dual information preserving method）方法

界面作为最为常见的物理现象之一，广泛的存在于力学、化学、生物工程、材料科学和计算机图形学等多个学科领域。界面的准确模拟对于多相流动、晶体生长、火焰的发展和传播等等很多方面的研究都有重要意义。

1.1　不同的界面类型和界面方法

界面方法最早可以追溯到 1958 年的洛斯 · 阿拉莫斯国家实验室发展的 Particle-In-Cell(PIC) 方法 [81, 111] 。关于不同的界面方法第一章 **??** 节中有较详细介绍。本章中，我们将从方程的角度来分析界面问题。

忽略力学模型，界面的运动可以抽象为求解对流方程

$$\frac{\partial z}{\partial t} + \boldsymbol{V} \cdot \nabla z = 0 \tag{1.1}$$

其中 $\boldsymbol{V}$ 为速度场，z 为区分界面两侧物质相关的量。下面分别对不同的界面类型进行分析。

1.1.1　传统界面

方程 (1.1) 尽管是最简单的对流方程，然而如果我们关注于界面运动时，想要实时的得到几何面（线）是异常困难的。以一维图 1.3 为例，如果直接对方程（1.1) 进行求解，例如采用差分方法，随着间断被耗散，界面将无法识别。

因此，绝大多数界面方法其实并不直接求解方程 (1.1) 本身，而是采用一种追踪的视角，图 1.2 给出不同界面方法的一维示意图。其中锋面追踪方法直接追踪界面；MAC 方法在界面一侧添加标记点；而 VOF 方法在每一个网格引入一个体积分数函数，将界面的运动转化为体积分数的变化。只有 level set 方法求解方程 (1.1)，但是也并不直接求解间断函数 z 本身，而是以到界面距离为函

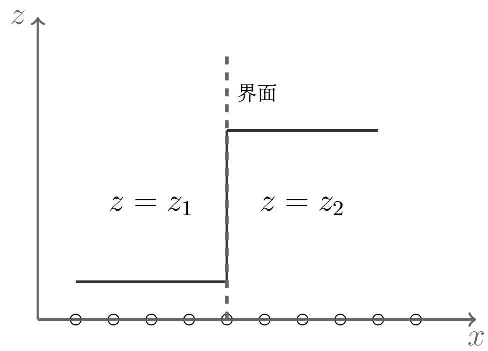


图 1.1: 界面的 1D 示意图

数构造一个新的光滑的 level set 函数 ϕ，求解

$$\frac{\partial \phi}{\partial t} + \boldsymbol{V} \cdot \nabla \phi = 0$$

如图 1.2.d 所示，level set 方法将 $\phi = 0$ 的位置识别为界面位置。

这些界面方法明显可以分成两类，一类全计算域计算的界面捕捉方法，如 VOF 和 level set 方法，另外一类只对部分区域进行 Lagrangian 追踪的界面追踪方法，如锋面追踪、MAC 方法等。两类方法各有优势，全域计算的方法更适合处理光滑的几何形状，并且易于处理由于由于流体压缩性导致的膨胀过程；Lagrangian 局部追踪的方法更易于处理锋利夹角、大变形以及界面破碎等问题。由于各有明显的优势和缺点，有学者尝试将两种类型方法结合发展如 level set-粒子方法，VOF-粒子方法等方法。

1.1.2 多相界面和耗散界面

除经常研究的两相界面外，在工业、化学、生物等很多领域中存在三相甚至更多相物质之间的相互作用，我们可以将这种问题称为多相界面问题。相比两相界面丰富的研究，多相界面的研究无论在理论还是数值方面都很少 [?]。耗散界面我们在第一章中做过简单介绍，和多界面类似，耗散界面同样也是较难处理的一类界面问题。

传统界面类方法求解多相界面和耗散界面困难的根本原因是由于这些方法都不是针对某一真实的物理量进行求解，如 γ，ρ，而只是从拓扑角度计算界面的运动。这一问题导致传统界面类方法无法直接求解如图 1.4 所示的多相界面

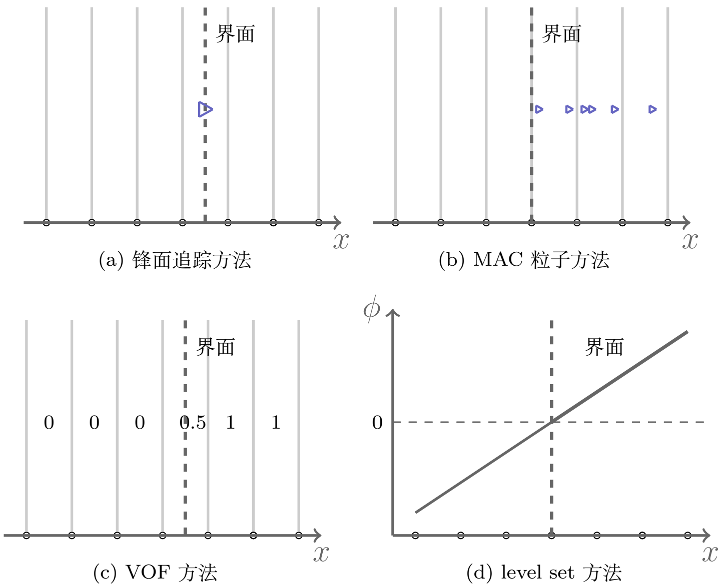


图 1.2: 不同界面方法 1D 示意图

和具有界面厚度 δ 的耗散界面。

1.2　双信息点方法基本思想

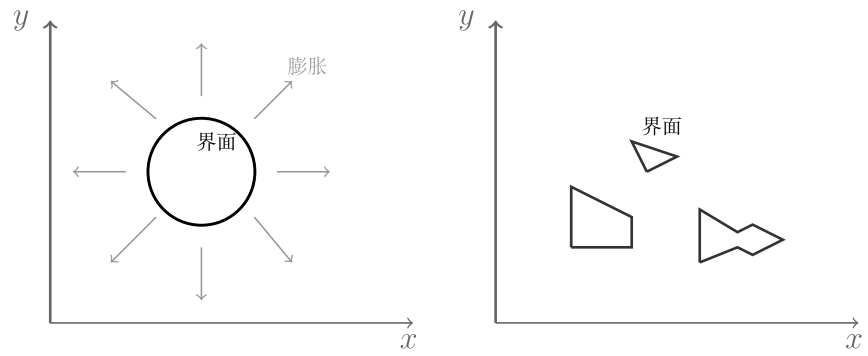
首先我们考虑两个问题，

1, 界面捕捉类方法由于采用全计算域求解，可以更好的处理界面膨胀（图 1.4.a ）、界面张力等光滑函数问题；界面追踪方法由于采用拉格朗日运动思想可以更好的保持界面形状、计算界面大变形和破裂等问题。我们能否同时具备两方面的优点?

2, 传统界面方法都不是直接求解方程（1.1）中的和物理相关的量 z ，因此较难处理多相界面和耗散界面。界面方法能否针对 z 直接求解?

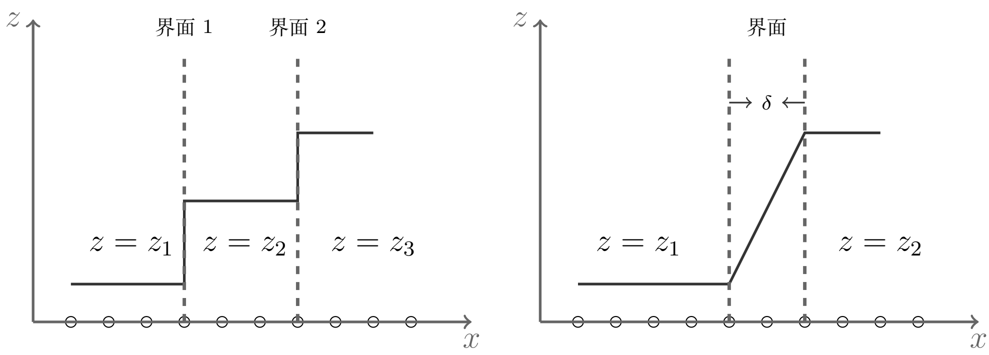
1.2.1　单元信息点

粒子方法是一种最直观的界面方法，具有优良的 Lagrangian 特性，但是由于它明显的不足导致学者们更愿意将它当成一种辅助的手段，如用作示踪粒子，或者和其它方法结合，如 level set-粒子方法，VOF-粒子方法等，用粒子修正界



(a) 界面捕捉方法 (b) 界面追踪方法

图 1.3: 不同类型界面方法适应的计算工况 2D 示意图



(a) 多相界面 1D 示意图 (b) 耗散界面 1D 示意图

图 1.4: 多相界面和耗散界面 1D 示意图

面的计算结果。粒子方法最大的问题是由于粒子的离散性，难以保证全计算域的覆盖，这样就无法像网格方法一样，随时得到确定位置的信息。

粒子类界面方法主要包括早期的 Particle-in-cell（PIC）方法和目前仍在使用的 Marker-in-Cell（MAC）方法。PIC 方法采用携带有质量的真实粒子模拟流体的运动，根据粒子携带的信息可以判断界面位置，然而，由于真实粒子无法人为的生成和抹去，无法保证全计算域每个网格都含有粒子。Marker-and-cell (MAC) 方法采用标记粒子，粒子除位置以外不含有其它信息，是完全的虚拟粒子，增加和减少都不会影响流场的物理性质，但是由于它完全不携带信息，只能通过有粒子和没有粒子判断界面，仍然无法做到覆盖计算域。

这里，我们引入一种新型粒子 — **信息点**，信息点上携带有对流的物理信息

z。不同于 PIC 中的真实粒子，信息点可以看成是对所在物理场的一种映射。其实网格同样是对真实场的一种映射，所以我们可以随时加密网格、减少网格甚至移动网格的位置，尽管这可能影响计算精度，但是并不会改变所研究问题本质。类比与网格，信息点同样是一种映射，我们可以根据需要增加、减少和移动。

第二章　化学反应中相关尺度的探讨

尺度在英文中对应于“scale”，而“scale”是一个较常用而且意义宽泛的名词和动词。作为名词，尺度主要包含以下两层含义：

1. 主观的度量，《Cambridge Dictionary》解释为“a set of numbers, amounts, etc., used to measure or compare the level of something”。在本文可以对应于网格尺度、时间步长，是我们主观观察问题所采用的度量的大小。

2. 客观事物特征与变化的空间和时间范围，《Cabridge Dictionary》解释为“the size or level of something”。文中对应于时间尺度、空间尺度和特征尺度等等。

2.1　化学反应时间尺度分析方程和空间尺度分析方程

除了对尺度概念简单的字面理解，在研究中，每种尺度都应该有更明确的数学定义。为了便于理解全文，下面对空间尺度和时间尺度进行简单的分析和解释，更准确、详细的理论工作请参阅 [102, 216]。

各种尺度的分析都是针对如下形式 ODE 方程展开的。

$$\frac{dY_i}{dx} = f_i(Y_1, Y_2, \cdots, Y_n) \tag{2.1}$$

对于化学反应时间尺度分析，采用反应 ODE 方程

$$\frac{dz_i}{dt} = \frac{\omega_i}{\rho_i}, \quad i = 1, \cdots, ns-1 \tag{2.2}$$

明显满足方程 (2.1) 的形式，

对于化学反应的空间尺度分析，我们需要对反应 Euler 方程做一些特殊的处理，以一维反应 Euler 方程为例

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = S \tag{2.3}$$

其中

$$U=\begin{pmatrix}\rho\\ \rho u\\ E\\ \rho z_1\\ \rho z_2\\ \vdots\\ \rho z_{ns-1}\end{pmatrix},F=\begin{pmatrix}\rho u\\ \rho u^2+p\\ u(E+p)\\ \rho z_1 u\\ \rho z_2 u\\ \vdots\\ \rho z_{ns-1}u\end{pmatrix},S=\begin{pmatrix}0\\ 0\\ 0\\ \omega_1\\ \omega_2\\ \vdots\\ \omega_{ns-1}\end{pmatrix},$$

跨过激波，如果采用随体坐标，流体满足如下形式方程

$$\begin{cases}\dfrac{d}{dx}(\rho u)=0\\ \dfrac{d}{dx}(\rho u^2+p)=0\\ \dfrac{d}{dx}[u(E+p)]=0\\ \dfrac{d}{dx}(\rho u z_i)=\omega_i,\quad i=1,\cdots,ns-1\end{cases}$$

如果假设波前的状态为

$$(\rho,u,p,z_i,E,T)=(\rho_0,D,p_0,z_{i0},E_0,T_0),\quad i=1,\cdots,ns-1$$

既可得到爆轰波的 Rankine-Hugoniot 关系

$$\rho u=\rho_0 D \tag{2.4}$$

$$\rho u^2+p=\rho_9 D^2+p_0 \tag{2.5}$$

$$E+p=E_0+p_0 \tag{2.6}$$

$$\frac{dz_i}{dx}=\frac{\omega_i}{\rho_i D},\quad i=1,\cdots,ns-1 \tag{2.7}$$

我们可以看到反映化学反应的时间尺度的方程 (2.2) 和空间尺度的方程 (2.7) 非常接近，实际上仅相差一个爆轰波波速 D。

2.2　尺度分析 [216]

我们对方程 (2.2) 进行经典的特征分析，为了方便我们将方程写为

$$\frac{d\boldsymbol{y}}{dx}=\boldsymbol{f}(\boldsymbol{y})$$

其中 $\boldsymbol{y}=(Y_1,\cdots,Y_n)$，$\boldsymbol{f}=(f_1,\cdots,f_n)$。然后，我们在点 $(x,\boldsymbol{y})=(x^*,\boldsymbol{y}^*)$ 进行线化处理

$$\frac{d\boldsymbol{y}}{dx}=\boldsymbol{J}\cdot(\boldsymbol{y}-\boldsymbol{y}^*)+\boldsymbol{b},\quad \boldsymbol{y}(x^*)=\boldsymbol{y}^* \tag{2.8}$$

其中 $\boldsymbol{J}=\partial f_i/\partial Y_j|_{y=y^*}$，而 $\boldsymbol{b}$ 为一个常数向量。

然后我们定义一个新量 $\zeta=\boldsymbol{y}-\boldsymbol{y}^*+\boldsymbol{J}^{-1}\cdot\boldsymbol{b}$，方程 (2.8) 变为

$$\frac{d\zeta}{dx}=\boldsymbol{J}\cdot\zeta,\quad \zeta(x^*)=\boldsymbol{J}\cdot\boldsymbol{b} \tag{2.9}$$

假设 $\boldsymbol{J}$ 是 n 维线性无关矩阵，可以将 $\boldsymbol{J}$ 特征分解为 $\boldsymbol{J}=\boldsymbol{P}\cdot\boldsymbol{\lambda}\cdot\boldsymbol{P}^{-1}$，假设 $\omega=\boldsymbol{P}^{-1}\cdot\zeta$，则上式可以化为

$$\frac{d\omega}{dx}=\Lambda\cdot\omega,\quad \omega(x^*)=\boldsymbol{P}^{-1}\cdot\boldsymbol{J}^{-1}\cdot\boldsymbol{b} \tag{2.10}$$

该方程的解为

$$\omega(x)=e^{\Lambda(x-x^*)}\cdot\boldsymbol{P}^{-1}\cdot\boldsymbol{J}^{-1}\cdot\boldsymbol{b} \tag{2.11}$$

第 i 项的当地 $x=x^*$ 特征尺度可以定义为

$$l_i=1/|\mathrm{Re}(\lambda_i)|, \tag{2.12}$$

对于方程 (2.7) 可以认为 l_i 为 i 组分的当地空间尺度 $\mathcal{L}_i$，对于方程 (2.2) 可以认为其为当地时间尺度 $\mathcal{T}_i$。同样我们可以定义，所有组分当地最小特征尺度为当地最佳空间尺度 $\mathcal{L}^{\mathrm{local}}$ 和当地最佳时间尺度 $\mathcal{T}^{\mathrm{local}}$。对于组分 i，全局最小的特征尺度可以定义为该组分的最佳空间尺度 $\mathcal{L}_i^{\mathrm{global}}$ 和最佳时间尺度 $\mathcal{T}_i^{\mathrm{global}}$。根据方程 (2.2) 和 (2.7) 关系我们可以推知 $\mathcal{L}_i^{\mathrm{global}}\propto D\mathcal{T}_i^{\mathrm{global}}$。由此我们也可以看出时间尺度和空间尺度间复杂的相关性。

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