1　4 次元変文データ同化

1.1　Cost Function

データ同化の定式化にあたり，コスト関数を

$$\mathcal{J}(\mathbf{v}, \mathbf{v}^0, \mathbf{V}) = \mathcal{D}(\mathbf{v}) + \mathcal{R}(\mathbf{v}^0, \mathbf{V}) \tag{1}$$

と定義する．ここで，右辺第 1 項は，計測速度と CFD 速度の誤差を表し

$$\mathcal{D}(\mathbf{v}) = \frac{\alpha}{2} \sum_{n=1}^{N} \sum_{m=1}^{M} \|\mathbf{v}_{\mathrm{CFD}} - \mathbf{v}_{\mathrm{MRI}}\|^2 \, \Delta x_{\mathrm{m}} \Delta y_{\mathrm{m}} \Delta z_{\mathrm{m}} \Delta t_{\mathrm{m}} \tag{2}$$

である．また，右辺第 2 項は，正則化項を表し

$$\mathcal{R}(\mathbf{v}^0, \mathbf{V}) = \frac{\beta}{2} \sum_{k=1}^{M} \int_{\Gamma_{\mathrm{I}}} \left(|\mathbf{V}|^2 + |\partial_s \mathbf{V}|^2 + \left|\dot{\mathbf{V}}\right|^2 + \left|\partial_s \dot{\mathbf{V}}\right|^2 \right) \mathrm{d}\Gamma + \frac{\gamma}{2} \int_{\Omega} \left(\left|\mathbf{v}^0\right|^2 + \left|\partial_s \mathbf{v}^0\right|^2 \right) \mathrm{d}\Omega \tag{3}$$

である．

1.2　Discretise-Then-Optimise Approach

流体の離散支配方程式を，ナビエ・ストークス方程式と連続の式を用いて

$$\frac{\mathbf{v}^{k+1} - \mathbf{v}^k}{\Delta t_{\mathrm{CFD}}} + \left(\frac{3}{2}\mathbf{v}^k - \frac{1}{2}\mathbf{v}^{k-1} \right) \cdot \nabla \mathbf{v}^{k+1/2} + \frac{1}{\rho} \nabla p^{k+1} - \nu \nabla^2 \mathbf{v}^{k+1/2} + \mathbf{K}(\phi) \mathbf{v}^{k+1/2} = \mathbf{0} \tag{4}$$

$$\nabla \cdot \mathbf{v}^{k+1} = \mathbf{0} \tag{5}$$

と記述する．ここで，移流項に対し 2 次精度 Adams-Bashforth 法，拡散項に対しては Crank-Nicolson 法を用いた．式 (4)，式 (5) に対し，重み付き残差法による弱形式を導き，全 CFD 時間ステップで総和を取ると，拘束条件が

$$\mathcal{F} = \sum_{k=0}^{N-1} \mathcal{F}_k = 0 \tag{6}$$

と表せる．ここで，

$$\begin{aligned} \mathcal{F}_k = &\int_{\Omega} \mathbf{w}^{k+1} \cdot \left(\frac{\mathbf{v}^{k+1} - \mathbf{v}^k}{\Delta t_{\mathrm{CFD}}} + \left(\frac{3}{2}\mathbf{v}^k - \frac{1}{2}\mathbf{v}^{k-1} \right) \cdot \nabla \mathbf{v}^{k+1/2} + \frac{1}{\rho} \nabla p^{k+1} - \nu \nabla^2 \mathbf{v}^{k+1/2} + \mathbf{K}(\phi) \mathbf{v}^{k+1/2} \right) \mathrm{d}\Omega \\ &+ \int_{\Omega} q^{k+1} (\nabla \cdot \mathbf{v}^{k+1}) \, \mathrm{d}\Omega - \int_{\Gamma_1} \lambda^{k+1} \cdot (\mathbf{v}^{k+1} - \mathbf{V}^{k+1}) \, \mathrm{d}\Gamma - \int_{\Gamma_1} \boldsymbol{\eta}^{k+1} \cdot \mathbf{w}^{k+1} \, \mathrm{d}\Gamma = 0 \end{aligned} \tag{7}$$

である．数値安定化手法に，SUPG/PSPG 法を用いたが，煩雑を避け，これらの項は省略する．さらに，目的関数・拘束条件を合わせた Lagrange 関数

$$\mathcal{L} = \mathcal{F} + \mathcal{J} \tag{8}$$

より，制約なし最小化問題を

$$\min_{\mathbf{v}^0, \mathbf{V}} \mathcal{L} \tag{9}$$

と定義する．

主問題は，

$$
{}^t\left\langle \frac{\partial \mathcal{L}}{\partial \mathbf{w}}, \tilde{\mathbf{w}} \right\rangle = \begin{pmatrix} \left\langle \frac{\partial \mathcal{L}}{\partial \mathbf{w}^1}, \tilde{\mathbf{w}}^1 \right\rangle \\ \vdots \\ \left\langle \frac{\partial \mathcal{L}}{\partial \mathbf{w}^N}, \tilde{\mathbf{w}}^N \right\rangle \end{pmatrix} = \mathbf{0}, \quad {}^t\left\langle \frac{\partial \mathcal{L}}{\partial q}, \tilde{q} \right\rangle = \begin{pmatrix} \left\langle \frac{\partial \mathcal{L}}{\partial q^1}, \tilde{q}^1 \right\rangle \\ \vdots \\ \left\langle \frac{\partial \mathcal{L}}{\partial q^N}, \tilde{q}^N \right\rangle \end{pmatrix} = \mathbf{0}, \quad {}^t\left\langle \frac{\partial \mathcal{L}}{\partial \boldsymbol{\lambda}}, \tilde{\boldsymbol{\lambda}} \right\rangle = \begin{pmatrix} \left\langle \frac{\partial \mathcal{L}}{\partial \boldsymbol{\lambda}^1}, \tilde{\boldsymbol{\lambda}}^1 \right\rangle \\ \vdots \\ \left\langle \frac{\partial \mathcal{L}}{\partial \boldsymbol{\lambda}^N}, \tilde{\boldsymbol{\lambda}}^N \right\rangle \end{pmatrix} = \mathbf{0} \tag{10}
$$

と表され，各時間ステップ k $(1 \le k \le N)$ において

$$
\begin{aligned}
\left\langle \frac{\partial \mathcal{L}}{\partial \mathbf{w}^k}, \tilde{\mathbf{w}}^k \right\rangle = \int_\Omega \Bigg(& \tilde{\mathbf{w}}^{k+1} \cdot \frac{\mathbf{v}^{k+1} - \mathbf{v}^k}{\Delta t_{\mathrm{CFD}}} + \tilde{\mathbf{w}}^{k+1} \cdot \left(\frac{3}{2}\mathbf{v}^k - \frac{1}{2}\mathbf{v}^{k-1} \right) \cdot \nabla \mathbf{v}^{k+1/2} + \frac{1}{\rho} p^{k+1} (\nabla \cdot \tilde{\mathbf{w}}^k) \\
& - \nu \nabla \tilde{\mathbf{w}}^{k+1} : \mathbf{v}^{k+1/2} + \tilde{\mathbf{w}}^{k+1} \cdot \mathbf{K}(\phi) \mathbf{v}^{k+1/2} \Bigg) \mathrm{d}\Omega - \int_{\Gamma_1} \boldsymbol{\eta}^{k+1} \cdot \tilde{\mathbf{w}}^{k+1} \, \mathrm{d}\Gamma = 0
\end{aligned} \tag{11}
$$

$$
\left\langle \frac{\partial \mathcal{L}}{\partial q^k}, \tilde{q}^k \right\rangle = \int_\Omega \tilde{q}^k (\nabla \cdot \mathbf{v}^{k+1}) \, \mathrm{d}\Omega = 0 \tag{12}
$$

$$
\left\langle \frac{\partial \mathcal{L}}{\partial \boldsymbol{\lambda}^k}, \tilde{\boldsymbol{\lambda}}^k \right\rangle = \int_{\Gamma_1} \tilde{\boldsymbol{\lambda}}^k \cdot (\mathbf{v}^{k+1} - \mathbf{V}^{k+1}) \, \mathrm{d}\Gamma = 0 \tag{13}
$$

とそれぞれ記述できる．

次に，随伴問題は，

$$
{}^t\left\langle \frac{\partial \mathcal{L}}{\partial \mathbf{v}}, \tilde{\mathbf{v}} \right\rangle = \begin{pmatrix} \left\langle \frac{\partial \mathcal{L}}{\partial \mathbf{v}^1}, \tilde{\mathbf{v}}^1 \right\rangle \\ \vdots \\ \left\langle \frac{\partial \mathcal{L}}{\partial \mathbf{v}^N}, \tilde{\mathbf{v}}^N \right\rangle \end{pmatrix} = \mathbf{0}, \quad {}^t\left\langle \frac{\partial \mathcal{L}}{\partial p}, \tilde{p} \right\rangle = \begin{pmatrix} \left\langle \frac{\partial \mathcal{L}}{\partial p^1}, \tilde{p}^1 \right\rangle \\ \vdots \\ \left\langle \frac{\partial \mathcal{L}}{\partial p^N}, \tilde{p}^N \right\rangle \end{pmatrix} = \mathbf{0}, \quad {}^t\left\langle \frac{\partial \mathcal{L}}{\partial \boldsymbol{\eta}}, \tilde{\boldsymbol{\eta}} \right\rangle = \begin{pmatrix} \left\langle \frac{\partial \mathcal{L}}{\partial \boldsymbol{\eta}^1}, \tilde{\boldsymbol{\eta}}^1 \right\rangle \\ \vdots \\ \left\langle \frac{\partial \mathcal{L}}{\partial \boldsymbol{\eta}^N}, \tilde{\boldsymbol{\eta}}^N \right\rangle \end{pmatrix} = \mathbf{0} \tag{14}
$$

と表され，各時間ステップ k $(1 \le k \le N)$ において

$$
\begin{aligned}
\left\langle \frac{\partial \mathcal{L}}{\partial \mathbf{v}^k}, \tilde{\mathbf{v}}^k \right\rangle = \int_\Omega \Bigg(& \frac{\mathbf{w}^k - \mathbf{w}^{k+1}}{\Delta t_{\mathrm{CFD}}} \cdot \tilde{\mathbf{v}}^k + \frac{1}{4}\mathbf{w}^k \cdot \left(3\mathbf{v}^{k-1} - \mathbf{v}^{k-2} \right) \cdot \nabla \tilde{\mathbf{v}}^k + \frac{3}{4}\mathbf{w}^{k+1} \cdot \tilde{\mathbf{v}}^k \cdot \nabla \mathbf{v}^{k+1} \\
& + \frac{1}{4}\mathbf{w}^{k+1} \cdot \left(3\mathbf{v}^k - \mathbf{v}^{k-1} \right) \cdot \nabla \tilde{\mathbf{v}}^k - \frac{1}{4}\mathbf{w}^{k+2} \cdot \tilde{\mathbf{v}}^k \cdot \nabla \mathbf{v}^{k+1} - \frac{1}{4}\mathbf{w}^{k+2} \cdot \tilde{\mathbf{v}}^k \cdot \nabla \mathbf{v}^k \\
& + q^{k+1} (\nabla \cdot \tilde{\mathbf{v}}^{k+1}) - \frac{1}{2}\nu \left(\nabla \mathbf{w}^k + \nabla \mathbf{w}^{k+1} \right) : \nabla \tilde{\mathbf{v}}^k + \frac{1}{2} \left(\mathbf{w}^k + \mathbf{w}^{k+1} \right) \cdot \mathbf{K}(\phi) \tilde{\mathbf{v}}^k \Bigg) \mathrm{d}\Omega \\
& + \int_{\Gamma_1} \lambda^{k+1} \cdot \tilde{\mathbf{v}}^k \, \mathrm{d}\Gamma + \alpha \sum_{i,j,k=1}^{M} (\mathbf{v}_{\mathrm{c}} - \mathbf{v}_{\mathrm{m}}) \, \tilde{\mathbf{v}} \Delta x_{\mathrm{m}} \Delta y_{\mathrm{m}} \Delta z_{\mathrm{m}} \Delta t_{\mathrm{m}} = 0
\end{aligned} \tag{15}
$$

$$
\left\langle \frac{\partial \mathcal{L}}{\partial p^k}, \tilde{p}^k \right\rangle = \int_\Omega \tilde{p}^k (\nabla \cdot \mathbf{w}^k) \, \mathrm{d}\Omega = 0 \tag{16}
$$

$$
\left\langle \frac{\partial \mathcal{L}}{\partial \boldsymbol{\eta}^k}, \tilde{\boldsymbol{\eta}}^k \right\rangle = \int_{\Gamma_1} \tilde{\boldsymbol{\eta}}^k \cdot \mathbf{w}^k \, \mathrm{d}\Omega = 0 \tag{17}
$$

とそれぞれ記述できる（Appendix A）．ここで，式（15）に関し

$$\begin{cases} \mathbf{v}^{k-2} = \mathbf{v}^0 & \text{for } k = 1 \\ \mathbf{w}^{k+2} = \mathbf{0} & \text{for } k = N-1 \\ \mathbf{w}^{k+1} = \mathbf{w}^{k+2} = \mathbf{0} & \text{for } k = N \end{cases} \tag{18}$$

である．

最後に，主問題，随伴問題より得た変数から，初期条件と，各時間ステップ k $(1 \leq k \leq N)$ における入口速度境界条件の感度

$$\begin{aligned} \left\langle \frac{\partial \mathcal{L}}{\partial \mathbf{v}^0}, \tilde{\mathbf{v}}^0 \right\rangle = \int_\Omega \Bigg(&- \frac{\mathbf{w}^1}{\Delta t_{\mathrm{CFD}}} \cdot \tilde{\mathbf{v}}^0 + \frac{3}{4}\mathbf{w}^1 \cdot \tilde{\mathbf{v}}^0 \cdot \nabla \mathbf{v}^1 + \frac{1}{2}\mathbf{w}^1 \cdot \mathbf{v}^0 \cdot \nabla \tilde{\mathbf{v}}^k - \frac{1}{4}\mathbf{w}^2 \cdot \tilde{\mathbf{v}}^0 \cdot \nabla \mathbf{v}^1 \\ &- \frac{1}{4}\mathbf{w}^2 \cdot \tilde{\mathbf{v}}^0 \cdot \nabla \mathbf{v}^0 - \frac{1}{2}\nu \nabla \mathbf{w}^1 : \nabla \tilde{\mathbf{v}}^0 + \frac{1}{2}\mathbf{w}^1 \cdot \mathbf{K}(\phi)\tilde{\mathbf{v}}^0 \Bigg) \mathrm{d}\Omega \end{aligned} \tag{19}$$

$$\left\langle \frac{\partial \mathcal{L}}{\partial \mathbf{V}^k}, \widetilde{\mathbf{V}}^k \right\rangle = \int_{\Gamma_{\mathrm{I}}} \beta \partial_s \mathbf{V}^k \cdot \widetilde{\mathbf{V}}^k + \lambda \cdot \widetilde{\mathbf{V}}^k \mathrm{d}\Gamma \tag{20}$$

を導出し，これらを用いて最適性条件

Appendix A　v に対するガトー微分

ラグランジュ関数の $\mathbf{v}$ でのガトー微分について，式 (14) のベクトル k 成分は,

$$\left\langle \frac{\partial \mathcal{L}}{\partial \mathbf{v}^k}, \tilde{\mathbf{v}}^k \right\rangle = \begin{cases} \left\langle \frac{\partial \mathcal{J}}{\partial \mathbf{v}^k}, \tilde{\mathbf{v}}^k \right\rangle + \left\langle \frac{\partial \mathcal{F}_{k-1}}{\partial \mathbf{v}^k}, \tilde{\mathbf{v}}^k \right\rangle + \left\langle \frac{\partial \mathcal{F}_{k}}{\partial \mathbf{v}^k}, \tilde{\mathbf{v}}^k \right\rangle + \left\langle \frac{\partial \mathcal{F}_{k+1}}{\partial \mathbf{v}^k}, \tilde{\mathbf{v}}^k \right\rangle & \text{for } 1 \leq k < N-1 \\ \left\langle \frac{\partial \mathcal{J}}{\partial \mathbf{v}^k}, \tilde{\mathbf{v}}^k \right\rangle + \left\langle \frac{\partial \mathcal{F}_{k-1}}{\partial \mathbf{v}^k}, \tilde{\mathbf{v}}^k \right\rangle + \left\langle \frac{\partial \mathcal{F}_{k}}{\partial \mathbf{v}^k}, \tilde{\mathbf{v}}^k \right\rangle & \text{for } k = N-1 \\ \left\langle \frac{\partial \mathcal{J}}{\partial \mathbf{v}^k}, \tilde{\mathbf{v}}^k \right\rangle + \left\langle \frac{\partial \mathcal{F}_{k-1}}{\partial \mathbf{v}^k}, \tilde{\mathbf{v}}^k \right\rangle & \text{for } k = N \end{cases} \tag{21}$$

であり，右辺はそれぞれ

$$\left\langle \frac{\partial \mathcal{J}}{\partial \mathbf{v}^k}, \tilde{\mathbf{v}}^k \right\rangle = \alpha \sum_{i,j,k=1}^{M} (\mathbf{v}_{\mathrm{c}} - \mathbf{v}_{\mathrm{m}})\, \tilde{\mathbf{v}} \Delta x_{\mathrm{m}} \Delta y_{\mathrm{m}} \Delta z_{\mathrm{m}} \Delta t_{\mathrm{m}} \tag{22}$$

$$\left\langle \frac{\partial \mathcal{F}_{k-1}}{\partial \mathbf{v}^k}, \tilde{\mathbf{v}}^k \right\rangle = \int_\Omega \left(\mathbf{w}^k \cdot \frac{\tilde{\mathbf{v}}^k}{\Delta t_{\mathrm{CFD}}} + \frac{1}{4}\mathbf{w}^k \cdot \left(3\mathbf{v}^{k-1} - \mathbf{v}^{k-2}\right) \cdot \nabla \tilde{\mathbf{v}}^k - \frac{1}{2}\nu \nabla \mathbf{w}^k : \nabla \tilde{\mathbf{v}}^k + \frac{1}{2}\mathbf{w}^k \cdot \mathbf{K}(\phi)\tilde{\mathbf{v}}^k \right) \mathrm{d}\Omega \tag{23}$$

$$\begin{aligned} \left\langle \frac{\partial \mathcal{F}_{k}}{\partial \mathbf{v}^k}, \tilde{\mathbf{v}}^k \right\rangle = \int_\Omega \Bigg(& \mathbf{w}^{k+1} \cdot \frac{-\tilde{\mathbf{v}}^k}{\Delta t_{\mathrm{CFD}}} + \frac{3}{4}\mathbf{w}^{k+1} \cdot \tilde{\mathbf{v}}^k \cdot \nabla \mathbf{v}^{k+1} + \frac{1}{4}\mathbf{w}^{k+1} \cdot \left(3\mathbf{v}^k - \mathbf{v}^{k-1}\right) \cdot \nabla \tilde{\mathbf{v}}^k \\ & - \frac{1}{2}\nu \nabla \mathbf{w}^{k+1} : \nabla \tilde{\mathbf{v}}^k + \frac{1}{2}\mathbf{w}^{k+1} \cdot \mathbf{K}(\phi)\tilde{\mathbf{v}}^k \Bigg) \mathrm{d}\Omega \end{aligned} \tag{24}$$

$$\left\langle \frac{\partial \mathcal{F}_{k+1}}{\partial \mathbf{v}^k}, \tilde{\mathbf{v}}^k \right\rangle = \int_\Omega \left(-\frac{1}{4}\mathbf{w}^{k+2} \cdot \tilde{\mathbf{v}}^k \cdot \nabla \mathbf{v}^{k+1} - \frac{1}{4}\mathbf{w}^{k+2} \cdot \tilde{\mathbf{v}}^k \cdot \nabla \mathbf{v}^k \right) \mathrm{d}\Omega \tag{25}$$

と表せる.