Model error in the rotating can

Elaine Spiller¹ and DW Han²

¹Marquette University ²University of Massachusetts at Amherst

February 12, 2013

Two models:

- kinematic3D velocity non-divergent but no dynamics
- CFD nonlinear numerical model, Navier-Stokes equations

Two models:

- kinematic3D velocity non-divergent but no dynamics
- CFD nonlinear numerical model, Navier-Stokes equations

Strategy:

- treat CFD as "reality" and take observations
- treat kinematic model as "model"

Two models:

- kinematic3D velocity non-divergent but no dynamics
- CFD nonlinear numerical model, Navier-Stokes equations

Strategy:

- treat CFD as "reality" and take observations
- treat kinematic model as "model"

Problem:

kinematic model can't reproduce CFD trajectories even with "best" choice of parameters

Two models:

- kinematic3D velocity non-divergent but no dynamics
- CFD nonlinear numerical model, Navier-Stokes equations

Strategy:

- treat CFD as "reality" and take observations
- treat kinematic model as "model"

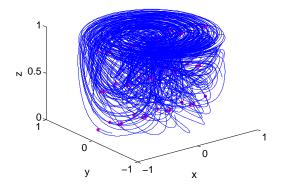
Problem:

 kinematic model can't reproduce CFD trajectories even with "best" choice of parameters

However:

 similar coherent structures (Poincaré sections and/or FTLEs) can be found in both systems

Trajectories from Tamay



- *u*, *v*, *w* from Navier Stokes with "wind" forcing
- Reynolds number, Re=100

Kinematic representation of velocity field

(Pratt and Rypina)

$$u(x, y, z) = -\frac{x}{3}(1 - 2z)(1 - r) - \alpha y - \frac{1}{2}\epsilon(1 - \beta z)(1 - r^2 - 2y^2)$$

$$v(x, y, z) = -\frac{y}{3}(1 - 2z)(1 - r) + \alpha x - \epsilon(1 - \beta z)xy$$

$$w(x, y, z) = z(1 - z)(\frac{2}{3} - r)$$

$$r^2 = x^2 + y^2$$

- lacktriangle non-divergent, satisfy no-normal flow bc at r=1, z=0,1
- lacksquare controls strength of horizontal velocity at origin
- lacksquare eta controls strength of vertical structure
- lacksquare lpha controls strength of horizontal swirling

Data = Model + Bias

$$Data = Model + Bias$$

$$Reality + Noise = Model + Bias$$

$$Data = Model + Bias$$

$$Reality + Noise = Model + Bias$$

CFD Simulation = Kinematic Model + Gaussian Process Model

$$Data = Model + Bias$$

$$Reality + Noise = Model + Bias$$

CFD Simulation = Kinematic Model + Gaussian Process Model

$$\mathbf{u}_{CFD}(x,y,z) = \mathbf{u}_{KM}(x,y,z,\alpha) + \mathbf{u}_{B}(x,y,z,\alpha)$$

OR

$$\mathbf{u}_{B}(x, y, z, \alpha) = \mathbf{u}_{CFD}(x, y, z, \alpha) - \mathbf{u}_{KM}(x, y, z)$$

■ input vector (*i* design points, *d* dimensions)

$$x_i = \{x_{i1}, ..., x_{id}\}$$

simulation response at design points

$$y_i(\mathbf{x}_i) = \beta + z(\mathbf{x}_i)$$

■ input vector (*i* design points, *d* dimensions)

$$x_i = \{x_{i1}, ..., x_{id}\}$$

simulation response at design points

$$y_i(\mathbf{x}_i) = \beta + z(\mathbf{x}_i)$$

■ treat y's as draws from a Gaussian process

mean
$$\beta$$
 $E[z(\mathbf{x}_i)] = 0$ $Var[z(\mathbf{x}_i)] = \sigma_z^2$

correlation structure

$$R_{ij} = corr[z(\mathbf{x}_i), z(\mathbf{x}_j)] = \prod_{k=1}^{a} exp\{-\theta_k(x_{ik} - x_{jk})^{1.9}\}$$

■ input vector (*i* design points, *d* dimensions)

$$x_i = \{x_{i1}, ..., x_{id}\}$$

simulation response at design points

$$y_i(\mathbf{x}_i) = \beta + z(\mathbf{x}_i)$$

- treat *y*'s as draws from a Gaussian process mean β $E[z(\mathbf{x}_i)] = 0$ $Var[z(\mathbf{x}_i)] = \sigma_z^2$
- correlation structure

$$R_{ij} = corr[z(\mathbf{x}_i), z(\mathbf{x}_j)] = \prod_{k=1}^{d} exp\{-\theta_k(x_{ik} - x_{jk})^{1.9}\}$$

■ untested point x̃

$$r_i(\tilde{\mathbf{x}}) = corr(z(\tilde{\mathbf{x}}), z(\mathbf{x}_i)), \qquad \mathbf{r} = (r_1(\tilde{\mathbf{x}}), ..., r_n(\tilde{\mathbf{x}}))'$$

■ input vector (*i* design points, *d* dimensions)

$$x_i = \{x_{i1}, ..., x_{id}\}$$

simulation response at design points

$$y_i(\mathbf{x}_i) = \beta + z(\mathbf{x}_i)$$

- treat *y*'s as draws from a Gaussian process mean β $E[z(\mathbf{x}_i)] = 0$ $Var[z(\mathbf{x}_i)] = \sigma_{\tau}^2$
- correlation structure

$$R_{ij} = corr[z(\mathbf{x}_i), z(\mathbf{x}_j)] = \prod_{k=1}^{d} exp\{-\theta_k(x_{ik} - x_{jk})^{1.9}\}$$

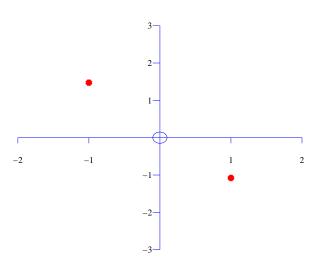
untested point x̄

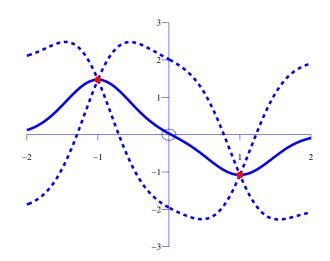
$$r_i(\tilde{\mathbf{x}}) = corr(z(\tilde{\mathbf{x}}), z(\mathbf{x}_i)), \qquad \mathbf{r} = (r_1(\tilde{\mathbf{x}}), ..., r_n(\tilde{\mathbf{x}}))'$$

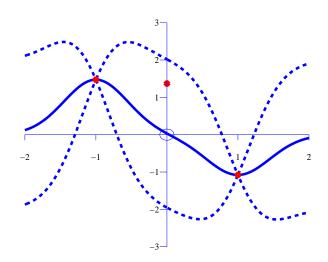
■ BLUP (mean and standard error)

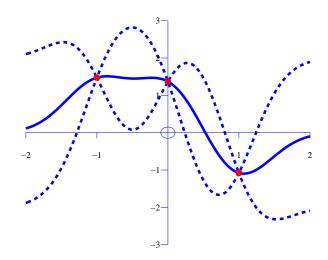
$$\hat{y}(\tilde{\mathbf{x}}) = \beta + \mathbf{r}' \mathbf{R}^{-1} (y(\tilde{\mathbf{x}}) - \beta)$$

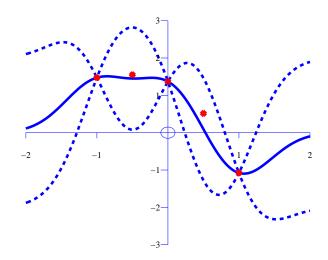
$$s^{2}(\tilde{\mathbf{x}}) = \sigma_{z}^{2}(1 - \mathbf{r}'\mathbf{R}^{-1}\mathbf{r}' + \frac{(1 - \mathbf{1}'\mathbf{R}^{-1}\mathbf{r}')^{2}}{\mathbf{1}'\mathbf{R}^{-1}\mathbf{1}'})$$

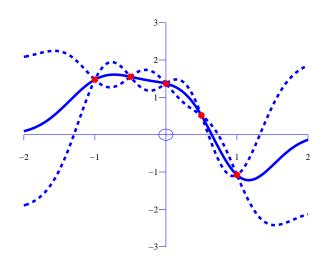












■ input vector $-(x, y, z, \alpha)$ evaluate $u_{CFD} - u_{KM}$ at N locations $\{(x_1, y_1, z_1, \alpha_1), (x_2, y_2, z_2, \alpha_2), \dots, (x_N, y_N, z_N, \alpha_N)\}$

- input vector $-(x, y, z, \alpha)$ evaluate $u_{CFD} u_{KM}$ at N locations $\{(x_1, y_1, z_1, \alpha_1), (x_2, y_2, z_2, \alpha_2), \dots, (x_N, y_N, z_N, \alpha_N)\}$
- response bias evaluated at input vector values, u_B
- \blacksquare treat u_B 's as draws from a Gaussian process

- input vector $-(x, y, z, \alpha)$ evaluate $u_{CFD} u_{KM}$ at N locations $\{(x_1, y_1, z_1, \alpha_1), (x_2, y_2, z_2, \alpha_2), \dots, (x_N, y_N, z_N, \alpha_N)\}$
- response bias evaluated at input vector values, u_B
- treat u_B's as draws from a Gaussian process
- correlation structure

$$\hat{R}_{i,j} = R((x_i, y_i, z_i, \alpha_i), (x_j, y_j, z_j, \alpha_j))$$

$$= \exp(-\theta_x |x_i - x_j|^{1.9} - \theta_y |y_i - y_j|^{1.9} - \theta_z |z_i - z_j|^{1.9} - \theta_\alpha |\alpha_i - \alpha_j|^{1.9})$$

- input vector $-(x, y, z, \alpha)$ evaluate $u_{CFD} u_{KM}$ at N locations $\{(x_1, y_1, z_1, \alpha_1), (x_2, y_2, z_2, \alpha_2), \dots, (x_N, y_N, z_N, \alpha_N)\}$
- response bias evaluated at input vector values, u_B
- treat u_B's as draws from a Gaussian process
- correlation structure

$$\hat{R}_{i,j} = R((x_i, y_i, z_i, \alpha_i), (x_j, y_j, z_j, \alpha_j))$$

$$= \exp(-\theta_x |x_i - x_j|^{1.9} - \theta_y |y_i - y_j|^{1.9} - \theta_z |z_i - z_j|^{1.9} - \theta_\alpha |\alpha_i - \alpha_j|^{1.9})$$

lacktriangle find $m{ heta}$'s that maximize $\mathcal{L}(m{ heta}) = p(\mathbf{u}_B | m{ heta}, \mathbf{x}, \mathbf{y}, \mathbf{z}, m{lpha})$

- input vector $-(x, y, z, \alpha)$ evaluate $u_{CFD} u_{KM}$ at N locations $\{(x_1, y_1, z_1, \alpha_1), (x_2, y_2, z_2, \alpha_2), \dots, (x_N, y_N, z_N, \alpha_N)\}$
- response bias evaluated at input vector values, **u**_B
- treat u_B's as draws from a Gaussian process
- correlation structure

$$\hat{R}_{i,j} = R((x_i, y_i, z_i, \alpha_i), (x_j, y_j, z_j, \alpha_j))$$

$$= \exp(-\theta_x |x_i - x_j|^{1.9} - \theta_y |y_i - y_j|^{1.9} - \theta_z |z_i - z_j|^{1.9} - \theta_\alpha |\alpha_i - \alpha_j|^{1.9})$$

- lacktriangle find $m{ heta}$'s that maximize $\mathcal{L}(m{ heta}) = p(\mathbf{u}_B | m{ heta}, \mathbf{x}, \mathbf{y}, \mathbf{z}, m{lpha})$
- untested scenario $-(\tilde{x}, \tilde{y}, \tilde{z}, \tilde{\alpha})$ not used as input
- how "close" is that scenario to those evaluated above

$$\hat{\mathbf{r}} = (R((\tilde{x}, \tilde{y}, \tilde{z}, \tilde{\alpha}), (x_1, y_1, z_1, \alpha_1)), \dots, R((\tilde{x}, \tilde{y}, \tilde{z}, \tilde{\alpha}), (x_N, y_N, z_N, \alpha_N)))^T$$

- input vector $-(x, y, z, \alpha)$ evaluate $u_{CFD} u_{KM}$ at N locations $\{(x_1, y_1, z_1, \alpha_1), (x_2, y_2, z_2, \alpha_2), \dots, (x_N, y_N, z_N, \alpha_N)\}$
- response bias evaluated at input vector values, **u**_B
- treat u_B's as draws from a Gaussian process
- correlation structure

$$\hat{R}_{i,j} = R((x_i, y_i, z_i, \alpha_i), (x_j, y_j, z_j, \alpha_j))$$

$$= \exp(-\theta_x |x_i - x_j|^{1.9} - \theta_y |y_i - y_j|^{1.9} - \theta_z |z_i - z_j|^{1.9} - \theta_\alpha |\alpha_i - \alpha_j|^{1.9})$$

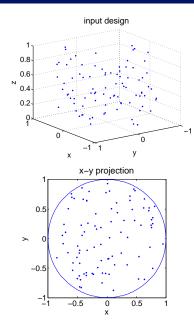
- find θ 's that maximize $\mathcal{L}(\theta) = p(\mathbf{u}_B | \theta, \mathbf{x}, \mathbf{y}, \mathbf{z}, \alpha)$
- untested scenario $-(\tilde{x}, \tilde{y}, \tilde{z}, \tilde{\alpha})$ not used as input
- how "close" is that scenario to those evaluated above

$$\hat{\mathbf{r}} = (R((\tilde{x}, \tilde{y}, \tilde{z}, \tilde{\alpha}), (x_1, y_1, z_1, \alpha_1)), \dots, R((\tilde{x}, \tilde{y}, \tilde{z}, \tilde{\alpha}), (x_N, y_N, z_N, \alpha_N)))^T$$

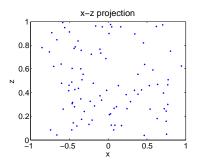
■ GaSP function – expected value of bias at the $(\tilde{x}, \tilde{y}, \tilde{z}, \tilde{\alpha})$

$$\hat{u}_B(\tilde{x}, \tilde{y}, \tilde{z}, \tilde{\alpha}) = \hat{\beta} + \hat{\mathbf{r}}^T \hat{\mathbf{R}}^{-1} (\mathbf{u}_B - \hat{\beta})$$

Strategy: design of inputs



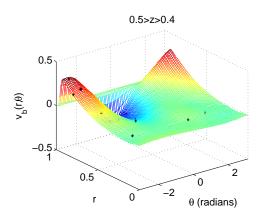
 data: sample CFD velocities at "spread out" locations around can (inputs)



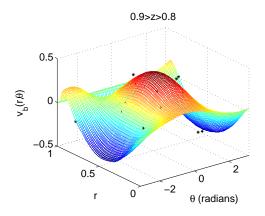
Strategy

- data: sample CFD velocities at "spread out" locations around can (inputs)
- evaluate kinematic model at input locations and calculate bias (responses)
- fit GaSP as model of bias for each u, v, w
- hard to fit, more natural w/inputs in cylindrical coordinates
 tricky, need periodic correlation (Spiller et al, submitted to SIAM JUQ)

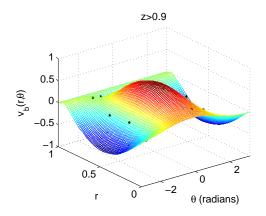
velocity bias at various depths



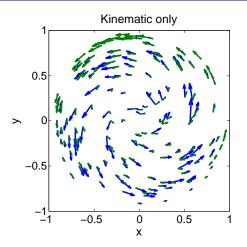
velocity bias at various depths



velocity bias at various depths

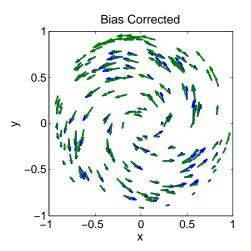


Comparison of velocity fields



- CFD field and "best fit" Kinematic field
- (u, v) projection of top of can, z > 0.8

Comparison of velocity fields



- CFD field and bias corrected kinematic field
- (u, v) projection of top of can, z > 0.8

Comparisons of trajectories

Kinematic model

$$\frac{dx}{dt} = u_{KM}, \quad \frac{dy}{dt} = v_{KM}, \quad \frac{dz}{dt} = w_{KM}$$

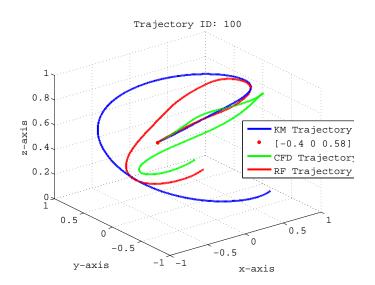
CFD model

$$\frac{dx}{dt} = u_{CFD}, \quad \frac{dy}{dt} = v_{CFD}, \quad \frac{dz}{dt} = w_{CFD}$$

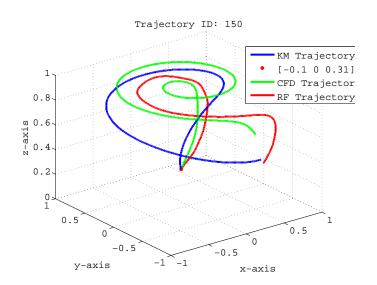
Bias corrected kinematic model (labeled RF)

$$\frac{dx}{dt} = u_{KM} + \hat{u}_{B}, \quad \frac{dy}{dt} = v_{KM} + \hat{v}_{B}, \quad \frac{dz}{dt} = w_{KM} + \hat{w}_{B}$$

Comparison of trajectories



Comparison of trajectories



Comparison of trajectories

