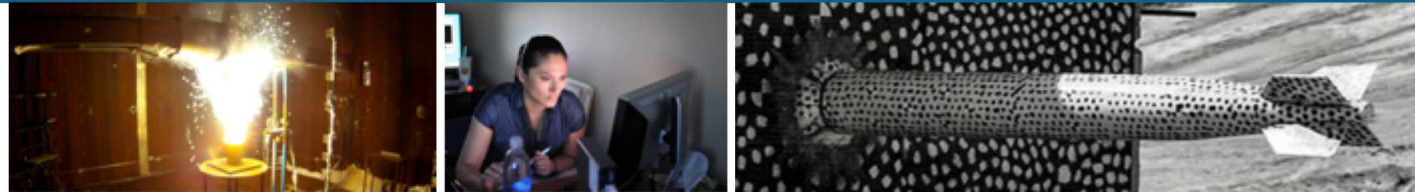




Sandia
National
Laboratories

SAND2020-6969C

WearGP: A UQ/ML wear prediction framework for slurry impellers and casings



¹SNL, ²GIW Industries, ³Georgia Institute of Technology

Anh Tran^{1,2}, Yan Wang³, John Furlan², Krishnan Pagalthivarthi², Mohamed Garman², Aaron Cutright², Robert Visintainer²

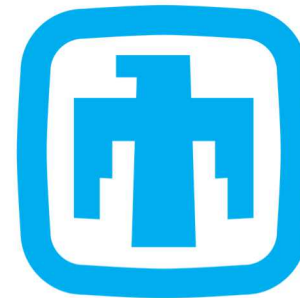


Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

2 Acknowledgement

Collaborators:

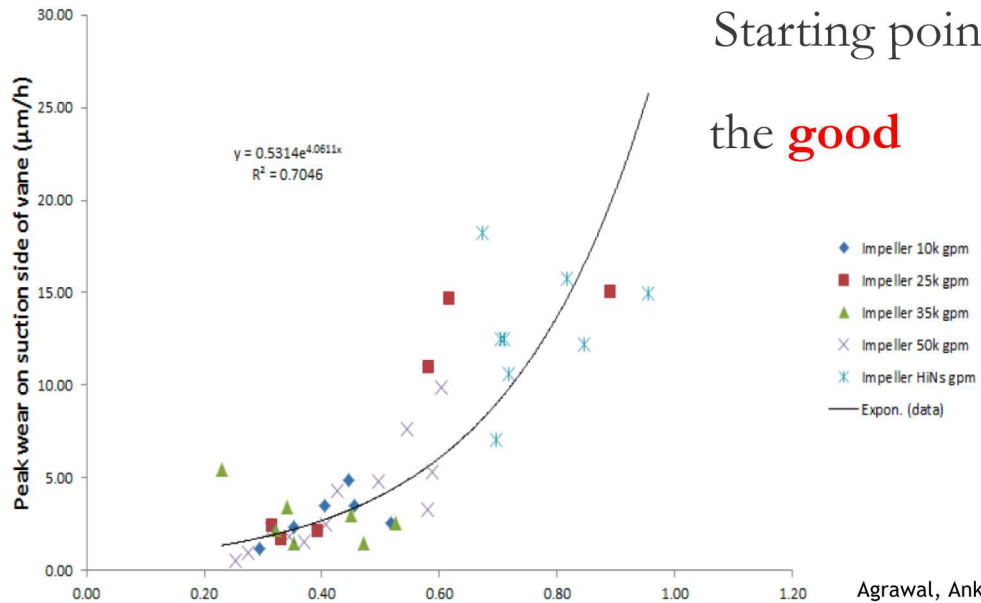
- GIW:
 - John Furlan †
 - Robert Visintainer
 - Krishnan Pagalthivarthi
 - Mohamed Garman
 - Aaron Cutright
- Georgia Tech:
 - Yan Wang
- SNL:
 - Tim Wildey



**Sandia
National
Laboratories**

Background

d50 = 300 μ m, Cv = 20%, TDH = 50m

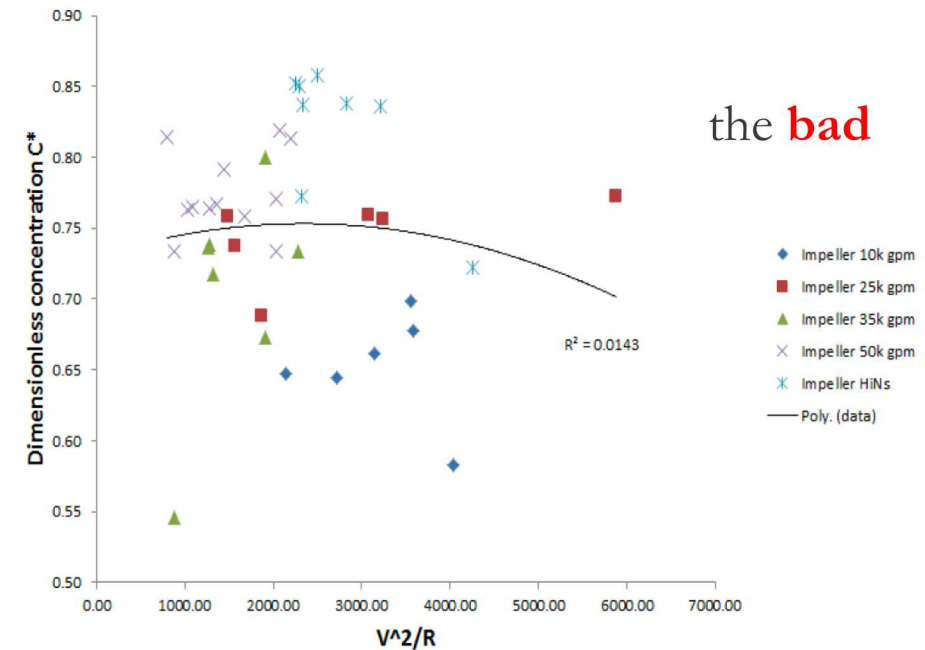


Starting point: 2013

the **good**

Agrawal, Ankit, and Alok Choudhary.
Apl Materials 4.5 (2016): 053208.

d50 = 300 μ m, Cv = 20%, TDH = 50m



the **bad**

... and the **frustrated intern**

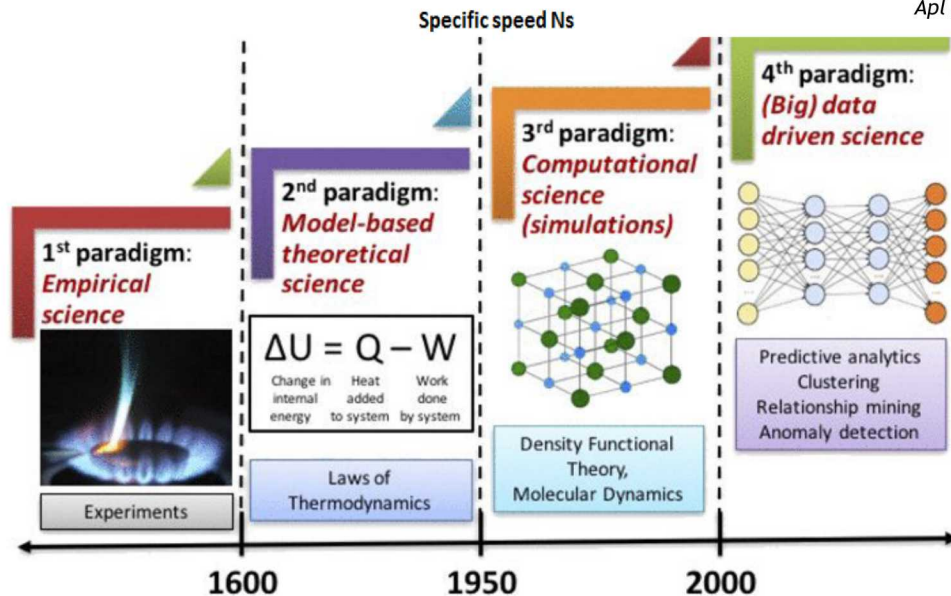
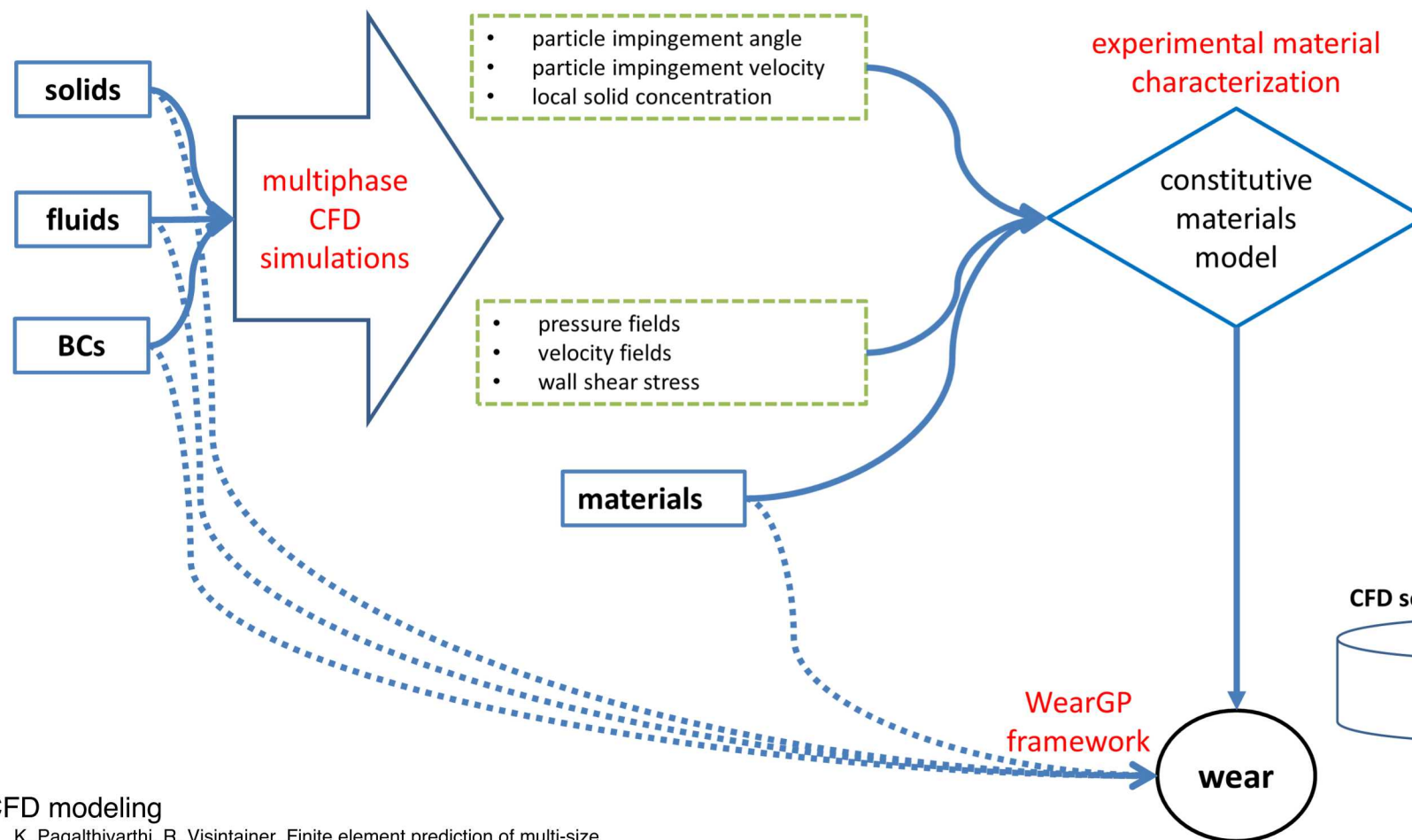


TABLE IV: Peak wear rate prediction for different surfaces with higher R^2

	Head coefficient ψ		Specific Diameter D_s		Specific Speed N_s	
	Prediction Equations	R^2	Predictions Equations	R^2	Predictions Equations	R^2
Shroud surface	$143.46e^{-31.79x}$	0.6541	$44.338x^{-1.74}$	0.5290	$1.075e^{2.8912x}$	0.5940
Hub surface	$294.25e^{-37.01x}$	0.4948	$97.425x^{-2.227}$	0.4835	$0.804e^{3.7727x}$	0.5644
pressure side of vane	$343.25e^{-42.39x}$	0.5268	$96.987x^{-2.552}$	0.5154	$0.4262e^{4.184x}$	0.5633
suction side of vane	$356.73e^{-41.28x}$	0.6632	$102.89x^{-2.475}$	0.6439	$0.5314e^{4.0611x}$	0.7046

TABLE V: Peak wear rate prediction for different surfaces with lower R^2

	Flow coefficient φ		Power coefficient C_p	
	Prediction Equations	R^2	Predictions Equations	R^2
Shroud surface	$1.8901e^{32.393x}$	0.4257	$851.3x^{0.8755}$	0.2637
Hub surface	$1.4783e^{46.914x}$	0.4982	$8281x^{1.2314}$	0.2911
pressure side of vane	$0.8488e^{51.523x}$	0.4876	$16875x^{1.4226}$	0.3153
suction side of vane	$1.0613e^{49.161x}$	0.5895	$14408x^{1.3694}$	0.3879

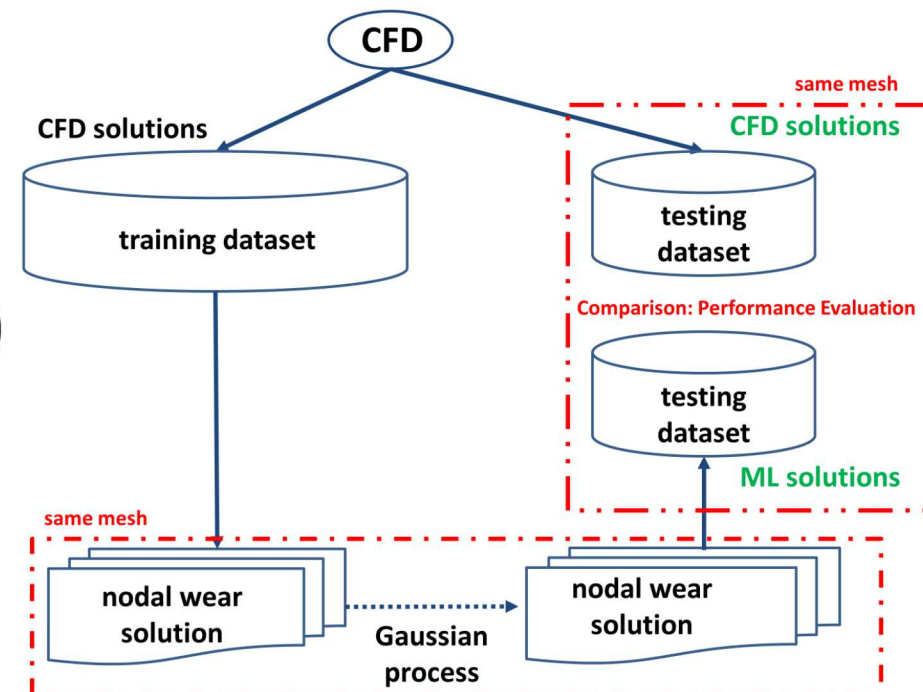


Calibration

- H.H. Tian, G.R. Addie, K.V. Pagalthivarthi, Determination of wear coefficients for erosive wear prediction through coriolis wear testing, *Wear* 259 (1–6) (2005) 160–170.
- K.V. Pagalthivarthi, J.M. Furlan, R.J. Visintainer, Consistent evaluation of wear coefficients from the experiments for use in CFD simulations, *ASME FEDSM* 2017.

UQVV – Experimental validation

- J.M. Furlan, V. Mundla, J. Kadambi, N. Hoyt, R. Visintainer, G. Addie, Development of A-scan ultrasound technique for measuring local particle concentration in slurry flows, *Powder Technol.* 215 (2012) 174–184
- Garman, M., Furlan, J. M., Globoke, W., Hoelling, M., Visintainer, R. J., Kadambi, J., Localized Particle Velocity and Concentration Measurement in Slurry Flow Using Ultrasound Technique. *ASME FEDSM* 2013.



CFD modeling

- K. Pagalthivarthi, R. Visintainer, Finite element prediction of multi-size particulate flow through three-dimensional channel: code validation, *J. Comput. Multiph. Flows* 5 (1) (2013) 57–72.
- K.V. Pagalthivarthi, R.J. Visintainer, Solid-liquid flow-induced erosion prediction in three-dimensional pump casing. *ASME FEDSM* 2009.
- K.V. Pagalthivarthi, J.M. Furlan, R.J. Visintainer, Finite element prediction of multi-size particulate flow through three-dimensional pump casing, *ASME FEDSM* 2015.
- K.V. Pagalthivarthi, J.M. Furlan, R.J. Visintainer, Wear rate prediction in multi-size particulate flow through impellers, *ASME FEDM* 2013.

$$\dot{W} = \dot{W}(\mathbf{x}_{\text{solids}}, \mathbf{x}_{\text{fluid}}, \mathbf{x}_{\text{BCs}}, \mathbf{x}_{\text{materials}})$$

ML

Tran, A., Furlan, J. M., Pagalthivarthi, K. V., Visintainer, R. J., Wildey, T., Wang, Y. (2019). WearGP: A computationally efficient machine learning framework for local erosive wear predictions via nodal Gaussian processes. *Wear*, 422, 9-26.

Training/testing dataset and GP

- 144 training data points
- 40 testing data points
- Very minimal for ML
- Fix a pump component, i.e. fix the geometric model
- Vary *all* BCs
- Regression of wear w.r.t. BCs
- Basis: (H, Q, d_{50}, C_v) .

$$\mathbf{f}|\mathbf{X} \sim \mathcal{N}(\mathbf{m}, \mathbf{K}),$$

$$\mathbf{y}|\mathbf{f}, \sigma^2 \sim \mathcal{N}(\mathbf{f}, \sigma^2 \mathbf{I}),$$

$$\mu_n(\mathbf{x}) = \mu_0(\mathbf{x}) + \mathbf{k}(\mathbf{x})^T (\mathbf{K} + \sigma^2 \mathbf{I})^{-1} (\mathbf{y} - \mathbf{m}),$$

$$\mathbf{K}_{i,j} = k(\mathbf{x}_i, \mathbf{x}_j) = \theta_0^2 \exp\left(-\frac{r^2}{2}\right), \quad \sigma_n^2 = k(\mathbf{x}, \mathbf{x}) - \mathbf{k}(\mathbf{x})^T (\mathbf{K} + \sigma^2 \mathbf{I})^{-1} \mathbf{k}(\mathbf{x}),$$

$$\log p(\mathbf{y}|\mathbf{x}_{1:n}, \theta) = -\frac{1}{2} \left(\mathbf{y} - \mathbf{m}_\theta^T \right) (\mathbf{K}^\theta + \sigma^2 \mathbf{I})^{-1} (\mathbf{y} - \mathbf{m}_\theta) - \frac{1}{2} \log |\mathbf{K}^\theta + \sigma^2 \mathbf{I}| - \frac{n}{2} \log(2\pi).$$

Parameters used for building training datasets.

Variable	Physical description	Unit	Lower bound	Upper bound	Used Values
H	pump head	m	35	65	35,50,65
%BEPQ	percentage of BEP flow rate	%	70	130	70,100,130
d_{50}	mean particle size	μm	150	600	150,300,450,600
C_v	concentration by volume	%	10	40	10,20,30,40

40 Testing cases and the corresponding operating conditions.

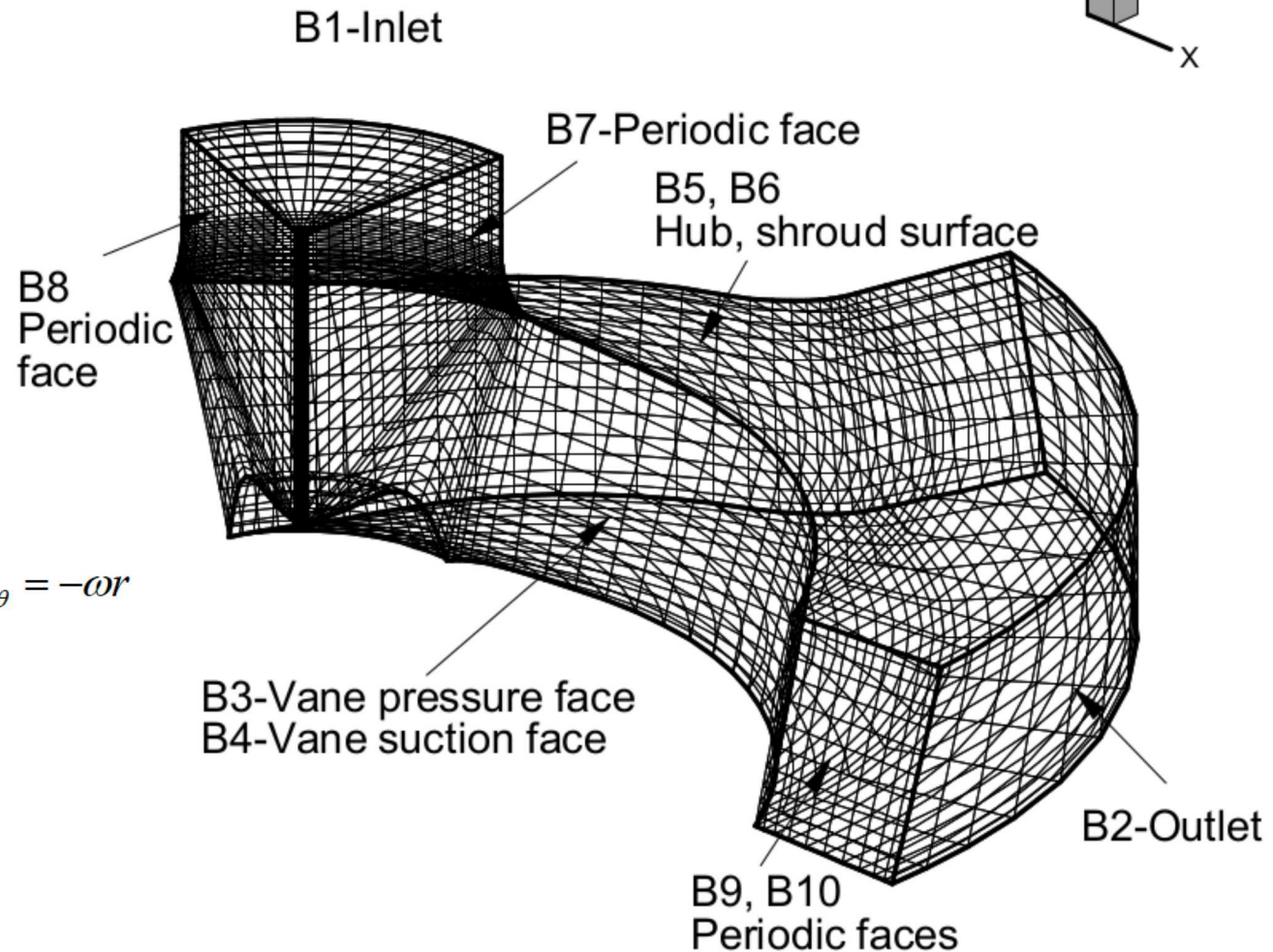
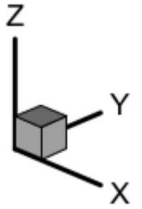
Testing case	H (m)	BEPQ (%)	d_{50} (μm)	C_v (%)
1	61.0238	100.7292	166.3271	17.1453
2	59.1267	98.1905	315.0980	32.1904
3	44.7113	108.3772	240.2366	20.7519
4	48.4715	91.1032	559.3353	30.8105
5	61.5799	88.8346	164.6182	29.2931
6	60.6776	93.6561	409.1707	14.3419
7	55.3361	90.3236	543.6216	30.1760
8	49.2122	79.0786	244.4687	33.3295
9	40.8413	96.6661	176.7400	18.0289
10	37.3730	84.1489	194.7891	23.2157
11	52.6503	89.6869	469.7961	35.7262
12	44.7080	95.1341	321.9043	38.8840
13	40.7969	79.9512	234.7505	12.2550
14	40.7849	84.3104	274.8115	34.8312
15	52.0627	86.1245	234.0740	38.4080
16	46.5643	106.2776	291.9244	36.7283
17	42.4220	91.7494	391.4051	36.8881
18	57.2903	89.4059	516.8324	36.8432
19	57.7757	81.3670	404.4440	14.4302
20	63.5732	77.5094	293.5427	18.2543
21	46.8153	105.3642	300.4395	21.8259
22	38.6464	76.4270	252.9711	29.3955
23	51.5555	94.2633	412.6286	19.7275
24	41.3691	81.1006	507.0509	30.9224
25	60.6506	105.4266	287.0631	31.1752
26	44.4207	99.7222	151.2729	29.2686
27	55.1794	76.4686	489.6172	21.6258
28	45.4443	80.8128	596.0691	10.3929
29	41.9834	81.6694	394.4312	21.1014
30	39.9178	105.8456	407.9843	36.4604
31	49.8985	86.2312	171.2106	28.1420
32	51.7241	93.4960	235.8800	35.4772
33	55.7365	79.2394	469.7201	39.0805
34	63.8825	77.7157	418.2133	39.7347
35	54.2585	106.0398	417.2460	29.2489
36	50.3763	85.9893	488.4799	32.5342
37	46.0812	90.4854	412.1844	24.4333
38	37.6830	87.7900	436.1273	22.7111
39	42.0202	96.4432	393.2446	16.7365
40	35.6735	94.1172	367.0682	11.8249



Solid-liquid CFD wear prediction – 3D Impeller



- Inlet velocity conditions on B1
- PBC on B7, B8, B9, B10
- Wall functions: B3, B4, B5, B6
- Stress-free condition on outlet B2



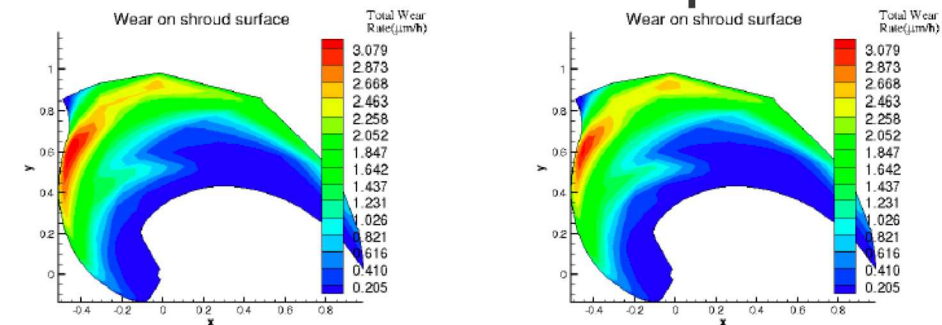
$$u_{l_z} = u_{m_z} = u_{k_z} = \frac{Q}{\pi R_1^2}, u_{l_r} = u_{m_r} = u_{k_r} = 0; u_{l_\theta} = u_{m_\theta} = u_{k_\theta} = -\omega r$$

$$C_k = C_{k,avg}, v_t = C_\mu^{0.25} \sqrt{\frac{3}{2}} U_0 T_i L, L = 0.14 R_2$$

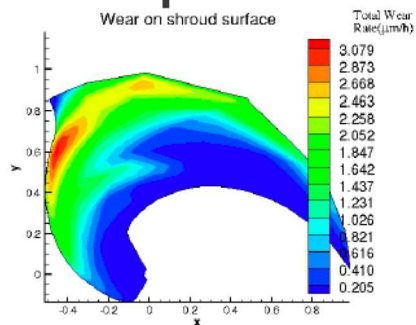
CFD modeling

K.V. Pagalthivarthi, J.M. Furlan, R.J. Visintainer, Wear rate prediction in multi-size particulate flow through impellers, ASME FEDM 2013.

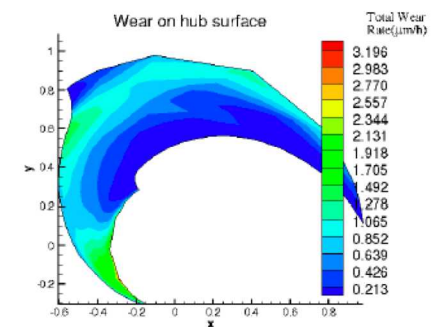
WearGP: 3D impeller showcases



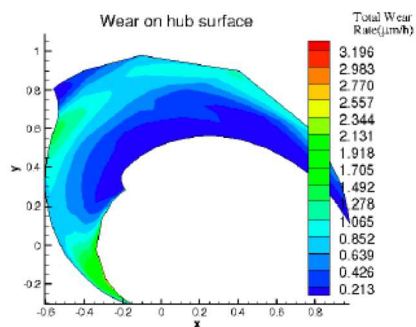
(a) CFD-3DImpeller: Shroud



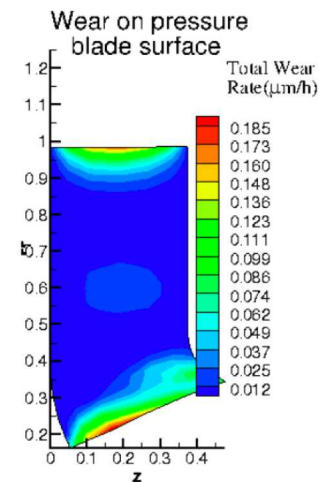
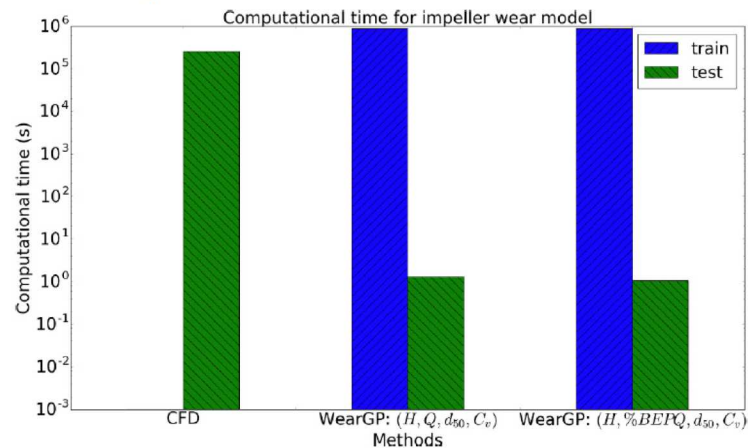
(b) WearGP: Shroud



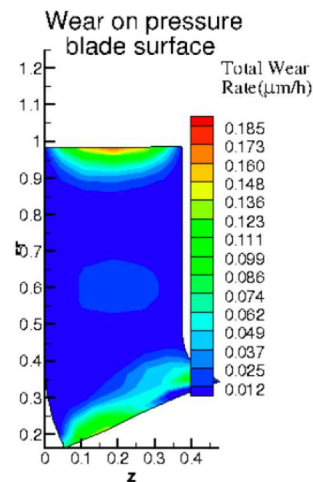
(c) CFD-3DImpeller: Hub



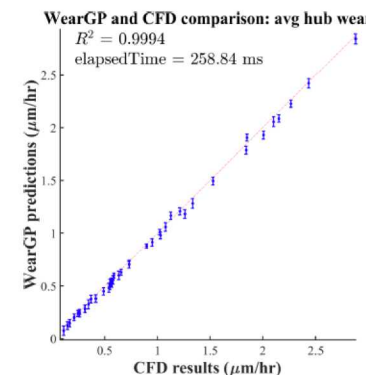
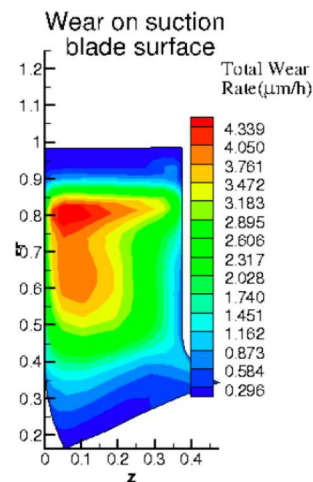
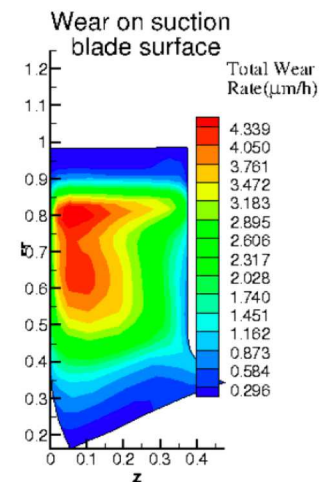
(d) WearGP: Hub



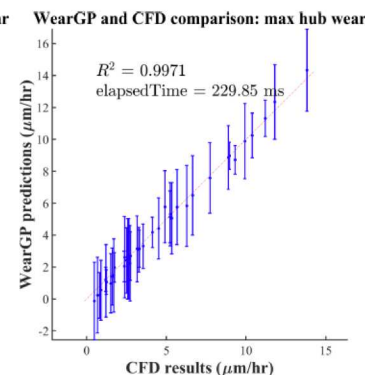
(e) CFD-3DImpeller: Pressure



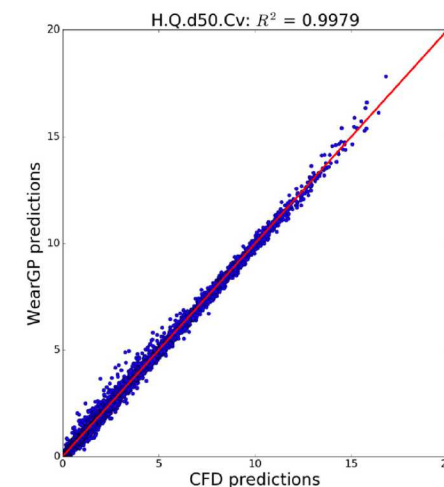
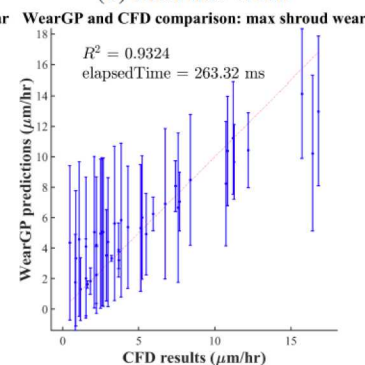
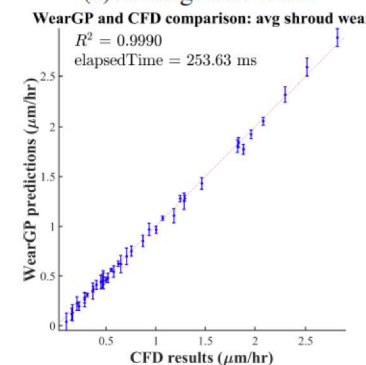
(f) WearGP: Pressure



(a) Average hub wear.



(b) Max hub wear.



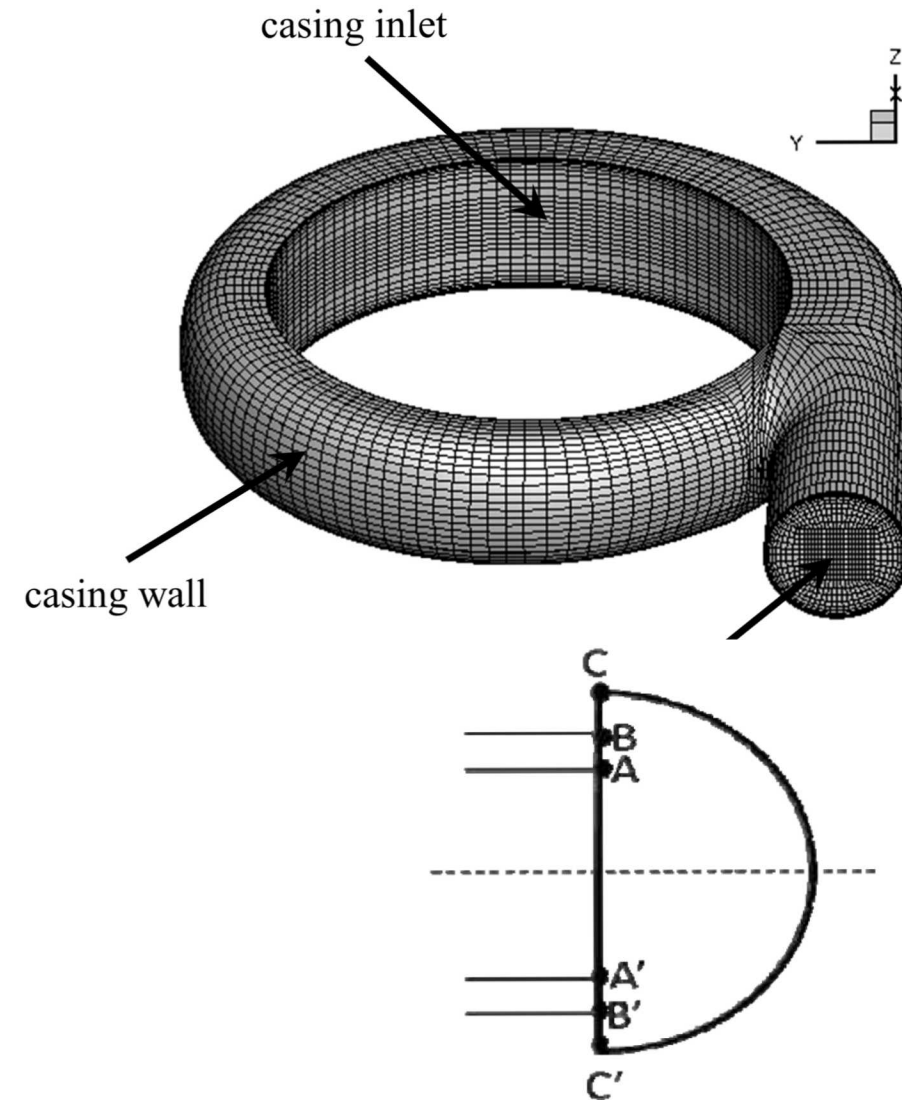
- Speedup:
 - Local: 234,134 x $\sim \mathcal{O}(10^5)$
 - Global: 976,659 x $\sim \mathcal{O}(10^6)$

- Inlet velocity conditions
- Wall functions
- Fully developed conditions at outlet:
 - Zero gradient for all fields except pressure in normal direction

$$u_{k_rad} = u_{m_rad} = u_{l_rad} = \frac{Q_m}{2\pi R_2 b}$$

$$u_{k_tan} = u_{m_tan} = u_{l_tan} = \frac{gH}{nU_\infty}, \quad C_k = C_{k,avg},$$

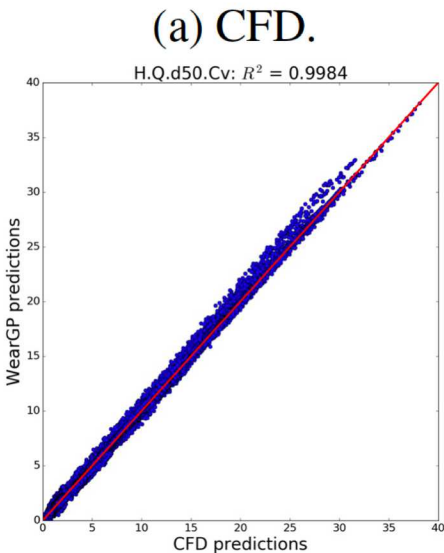
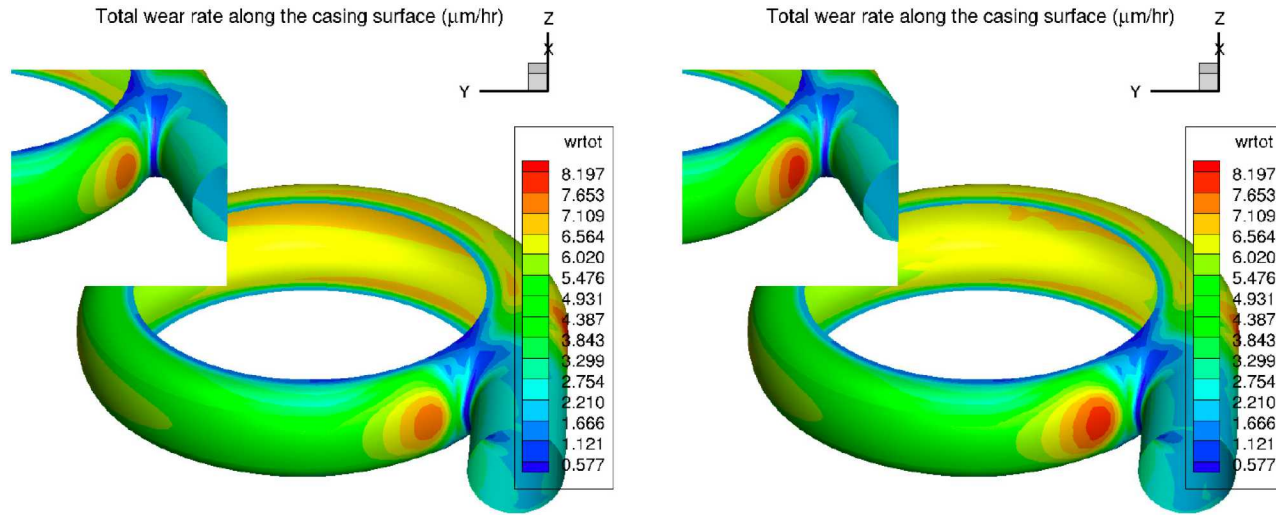
$$v_t = C_\mu^{0.25} \sqrt{\frac{3}{2}} U_0 T_i L, \quad L = 0.14 R_2$$



CFD modeling

- K.V. Pagalthivarthi, R.J. Visintainer, Solid-liquid flow-induced erosion prediction in three-dimensional pump casing. ASME FEDSM 2009.
- K.V. Pagalthivarthi, J.M. Furlan, R.J. Visintainer, Finite element prediction of multi-size particulate flow through three-dimensional pump casing, ASME FEDSM 2015.

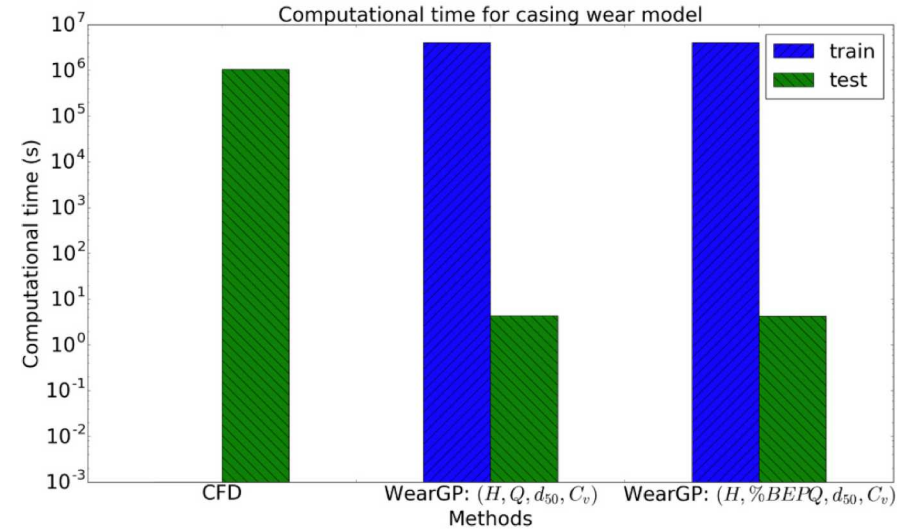
WearGP: 3D casing showcases



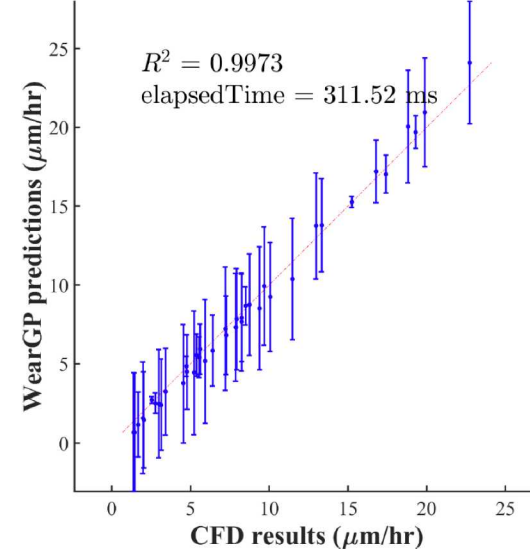
The left top corner is the zoom in view near the tongue region

(b) WearGP.

- Speedup:
 - Local: $247,985 \times \sim \mathcal{O}(10^5)$
 - Global: $3,406,532 \times \sim \mathcal{O}(10^6)$

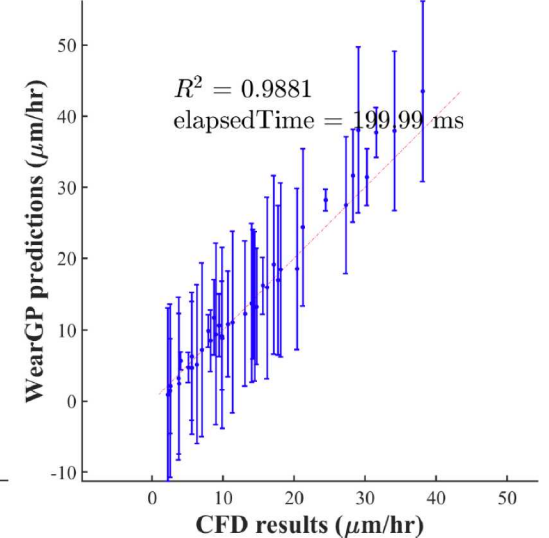


WearGP and CFD comparison: avg wear



(a) Average casing wear.

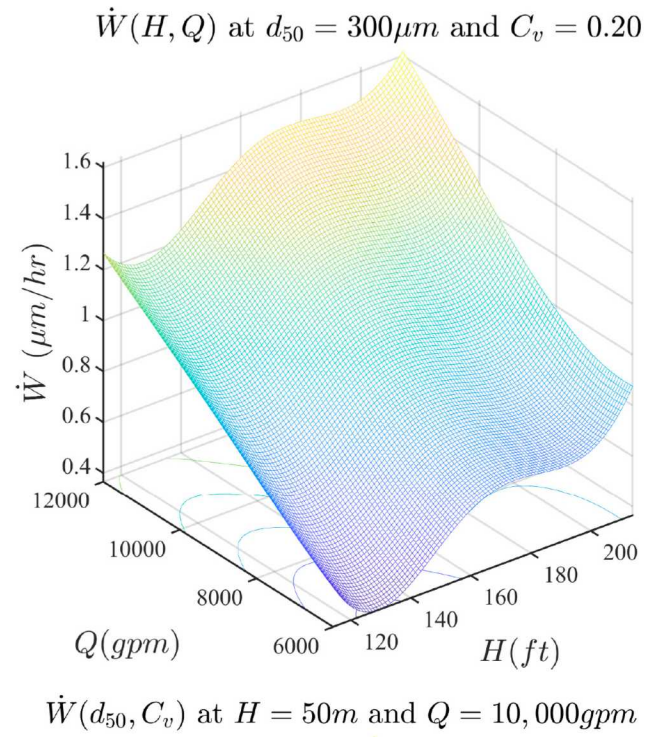
WearGP and CFD comparison: max wear



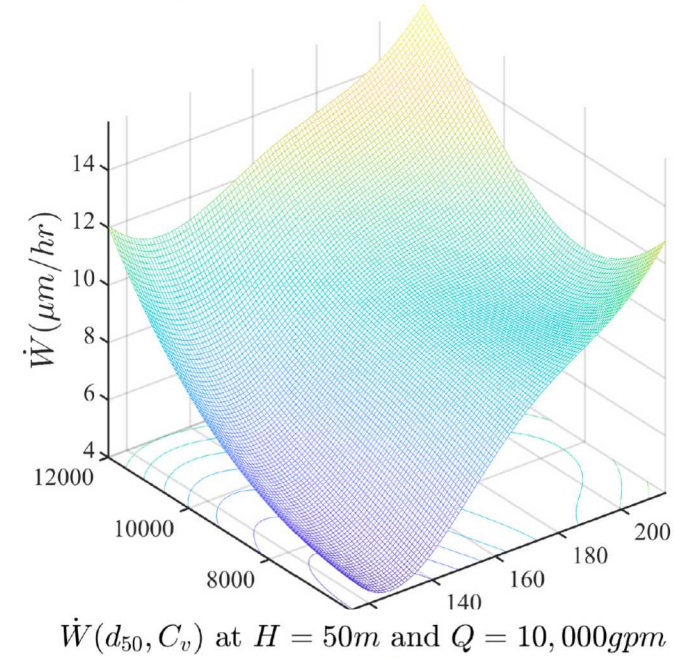
(b) Max casing wear.

Effects of X

Impeller



$$\dot{W}(H, Q) \text{ at } d_{50} = 300\mu m \text{ and } C_v = 0.20$$



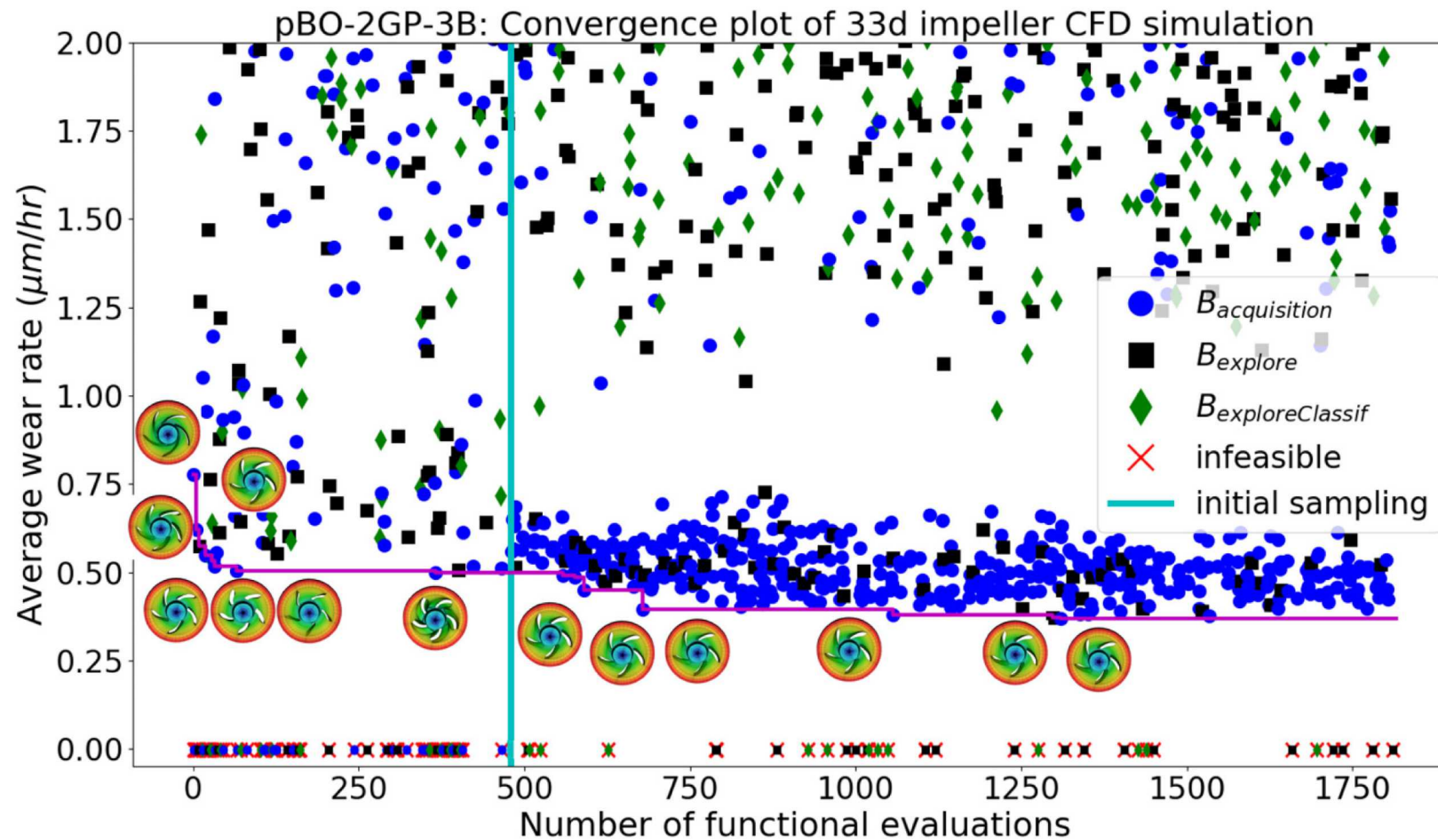
Casing



What if the geometric model changes?

- Can we change from one pump to another pump?
- Rephrase: can we change the design (parameters)?
- Yes, and we can even optimize the design using Bayesian optimization in parallel.

Tran, A., Sun, J., Furlan, J. M., Pagalthivarthi, K. V., Visintainer, R. J., Wang, Y. (2019). pBO-2GP-3B: A batch parallel known/unknown constrained Bayesian optimization with feasibility classification and its applications in computational fluid dynamics. Computer Methods in Applied Mechanics and Engineering, 347, 827-852.





Thank you for your listening. If you have any questions, please email: anhtran@sandia.gov