Robust optimization for Dense Gas Flows

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BACCHUS Team
AQUARIUS Associated Team

CTR, Stanford University
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AQUARIUS ASSOCIATED TEAM

- Partners: Bacchus Team (INRIA) + UQ LAB and CFG (STANFORD)
- Mission: collaborative works, joint projects on UQ and high-Reynolds number flows
- Supported by INRIA and INRIA@SyliconValley program
- Fellowships and scholarships to faculty, postdocs and graduate students
- WORKSHOP May 23-24 Berkeley Campus
Plan

- Why Organic Rankine Cycles?
- Issues for a predictive numerical simulation.
- Why uncertainties are so important?
- Just few concepts of thermodynamics
- Uncertain shape optimisation for dense gas flows
Organic Rankine Cycles (ORC)

Characteristics of low-power plants

- Use of organic working fluids instead of steam
- Very few (1 or 2) expansion stages
- Use of an impulse turbine (or a low-reaction turbine)

Advantages

- Fluids of retrograde type as working fluids
- Very high turbine efficiency (up to 85%) for $T_{\text{BOILER}} < 900\, \text{K}$
- Long life and Minimum maintenance requirements
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Exploitation of Renewable Sources
Organic Rankine Cycles (ORC)

Major loss mechanisms in transonic/supersonic turbomachinery

- Drop in Carnot Efficiency due to lower temperature ratio
- Shock waves
- Shock/boundary-layer interactions

Possible Solutions

- Use of peculiar fluids for which compression shocks are inadmissible
- Appropriate shape optimization of the blades

BZT FLUIDS + Optimization
Dense Gas Dynamics

- Study of the dynamic behavior of gases at pressures/densities of the order of magnitude of the liquid/vapor critical point

- The perfect gas law is replaced by more complex EOS:
  - van der Waals, Redlich-Kwong, Martin-Hou, ...
**Fundamental Derivative** of Gasdynamics:

\[
\Gamma = 1 + \frac{\rho}{a} \left( \frac{\partial a}{\partial \rho} \right)_s = \frac{v^3}{2a^2} \left( \frac{\partial^2 p}{\partial v^2} \right)_s \quad \left( a^2 = -v^2 \left( \frac{\partial p}{\partial v} \right)_s \right)
\]

**Perfect polytropic gases:** \( \Gamma = \frac{\gamma + 1}{2} > 1 \)

More complex fluids: \( \Gamma < 1 \rightarrow \) speed of sound decreases with rising pressure

\[
\Gamma = 1 + \frac{\rho}{a} \left( \frac{\partial a}{\partial \rho} \right)_s < 1 \quad \Leftrightarrow \quad \left( \frac{\partial a}{\partial \rho} \right)_s < 0
\]

**Fluids with** \( \Gamma < 0 \): Bethe-Zel’dovich-Thompson (BZT) fluids

- Region with \( \Gamma < 0 \): inversion zone
- \( \Gamma = 0 \) contour: transition line
Dense Gases
Inviscid properties

Bethe-Zel’dovich-Thompson Fluids (BZT)

- Several fluids normally used for the heat transfer have these properties
- Examples of BZT fluids:
  - Heavy Hydrocarbon
  - Heavy Fluorocarbons (PP10, PP11)
  - Any aromatic carbons
  - Any siloxanes
Dense Gases: Inviscid properties

- Entropy change across a weak shock:

\[
\Delta s = - \frac{a^2 \Gamma (\Delta v)^3}{v^3 6T} + O((\Delta v)^4),
\]

- If \( \Gamma < 0 \) (Inversion zone): compression shocks forbidden, expansion shocks admissible, mixed shock/fan waves, sonic shocks
  \( \rightarrow \) Non classical hyperbolic behaviors
- \( |\Gamma| < < 1 \) (\( \Gamma = O(\Delta v) \)) \( \rightarrow \) Entropy change one order lower than normal:
  \( \rightarrow \) reduced losses (1)
Interest of Dense Gases

Organic Rankine Cycles

- Retrograde fluids $\rightarrow$ superheat (become drier) when expanded
- More higher efficiency for low-power applications
- Typically work at transonic/supersonic flow conditions
  - Losses reduction due to shock waves and shock/boundary layer interaction
Interest of Dense Gases

Organic Rankine Cycles

- Rankine Cycles using heavy organic compounds instead of water
  - Retrograde fluids: superheat (become drier) when expanded
  - More higher efficiency for low-power applications
  - Typically work at transonic/supersonic flow conditions

AIM: DESIGN OF AN OPTIMAL BLADE TO MAXIMIZE PERFORMANCE

- Losses reduction due to shock waves and shock/boundary layer interaction
Sources of physical uncertainties in dense gas flows

2 physical sources of uncertainties

[Diagram of a closed-loop system with labeled components: 1) Condenser, 2) Pump, 3) Heater, 4) Turbine, with flow paths and heat transfer symbols.]
Sources of physical uncertainties in dense gas flows

2 physical sources of uncertainties

Difficulty to measure physical properties
- molecularly complex fluids
- close to the saturation curve
Sources of physical uncertainties in dense gas flows

2 physical sources of uncertainties

Difficult to measure physical properties
- molecularly complex fluids
- close to the saturation curve

Uncertain Inlet conditions because of variable heat sources
Necessity to optimize the turbine blade to exploit dense gas effects for the fluid considered and for the associated operating points taking into account uncertainties.
Shape optimization

- Necessity to optimize the turbine blade to exploit dense gas effects for the fluid considered and for the associated operating points taking into account uncertainties

1° source of uncertainty: thermodynamic model

2° source of uncertainty: inlet conditions

Necessity to optimize the turbine blade to exploit dense gas effects for the fluid considered and for the associated operating points taking into account uncertainties.

1° source of uncertainty: thermodynamic model

2° source of uncertainty: inlet conditions

3° source of Uncertainty: geometric tolerances

Uncertain shape optimization for dense gas flows

- **Objective**: Taking into account the physical and geometric sources of uncertainty to perform a shape optimization in dense gas flows
Uncertain shape optimization for dense gas flows

- **Objective**: Taking into account the physical and geometric sources of uncertainty to perform a shape optimization in dense gas flows

3 distinct sources of uncertainty
Uncertain shape optimization for dense gas flows

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Thermodynamic model
Uncertain shape optimization for dense gas flows

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3 distinct sources of uncertainty

- Thermodynamic model
- Geometry
Uncertain shape optimization for dense gas flows

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3 distinct sources of uncertainty

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- Geometry
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Few notions of thermodynamics

Let us consider Euler equations 1D

\[ w_t + f(w)_x = 0 \]

where \( w = (\rho, \rho u, \rho E)^T = (w_1, w_2, w_3)^T; \]

\[ f(w) = (\rho u, \rho u^2 + p(w), \rho uH(w))^T \]

\( \rho \) is the density, \( u \) velocity, \( E \) specific total energy, \( p \) pressure and \( H \) specific total enthalpy

Jacobian:

\[
A = \begin{pmatrix}
0 & 1 & 0 \\
\frac{\partial p}{\partial w_1} - u^2 & \frac{\partial p}{\partial w_2} + 2u & \frac{\partial p}{\partial w_3} \\
\left(\frac{\partial p}{\partial w_1} - H\right)u & H + \frac{\partial p}{\partial w_2}u & \left(1 + \frac{\partial p}{\partial w_3}\right)u
\end{pmatrix}.
\]

NEED FOR A RELATION TO CLOSE THE SYSTEM !!!

\[ p = p(w) \]
Few notions of thermodynamics

- van der Waals model
  \[ p = (\gamma - 1) \frac{\rho e + \alpha \rho^2}{1 - b \rho} - \alpha \rho^2 \]
  \( \rightarrow \) explicit relation \( p = p(w) \)

- Martin-Hou model
  - Thermal equation of state
    \[ p = \frac{RT}{\nu - b} + \sum_{i=2}^{5} \frac{f_i(T)}{(\nu - b)^i} \]
    \[ f_i(T) = A_i + B_i T + C_i e^{-\frac{kT}{T_c}} \]
  - Power law for ideal-gas specific heat
    \[ c_{\nu\infty}(T) = c_{\nu\infty}(T_c) \left( \frac{T}{T_c} \right)^n \]
Few notions of thermodynamics

- **Span-Wagner equation**
  - **Helmotz energy**

\[
\psi (\tau, \delta) = \psi^{0} (\tau, \delta) + \psi^{x} (\tau, \delta) \\
= \psi^{0} (\tau, \delta) + n_{1} \delta \tau^{0.250} + n_{2} \delta \tau^{-1.125} + n_{3} \delta \tau^{-1.500} \\
+ n_{4} \delta^{2} \tau^{1.375} + n_{5} \delta^{3} \tau^{-0.250} + n_{6} \delta^{7} \tau^{-0.875} \\
+ n_{7} \delta^{2} \tau^{0.625} e^{-\delta} + n_{8} \delta^{5} \tau^{1.750} e^{-\delta} + n_{9} \delta \tau^{3.625} e^{-\delta^{2}} \\
+ n_{10} \delta^{4} \tau^{3.625} e^{-\delta^{2}} + n_{11} \delta^{3} \tau^{14.5} e^{-\delta^{3}} + n_{12} \delta^{4} \tau^{12.0} e^{-\delta^{3}}
\]

\(\delta, \tau \rightarrow\) reduced density and temperature

- **\(n_{i}\) \rightarrow equation coefficients**
How considering Uncertainty on thermodynamic model?

- Uncertainty on the critical parameters of two equations, Redlich-Kwong, and Martin-Hou

\[
p = \frac{RT}{v-b} - \frac{a}{T^{0.5}} \frac{1}{v(v+b)}
\]

3 physical parameters → 3 uncertainties
\(\omega, c_{v\infty}(T_c)/R, n\)

\[
p = \frac{RT}{v-b} + \sum_{i=2}^{5} \frac{f_i(T)}{(v-b)^i}
\]

6 physical parameters physiques → 6 uncertainties
\(T_c, p_c, V_c, \omega, c_{v\infty}(T_c)/R, n\)

- Results:
  - Sensitivity of thermodynamic model to uncertainties on physical parameters → investigation over several parameters for airfoil \((C_L, C_D \ldots)\) and turbines (efficiency, power ...)
Uncertainty on thermodynamic model

- Dense gas flow over an airfoil, statistics on $C_D$, $D_5$ fluid

- Comparison between different equations of state
- Simple models are predictive and robust as well as the best accurate equations of state
Feasibility study

- A simpler configuration is considered ➔ a symmetric profile, $M_\infty=0.95$ and $0^\circ$ angle of attack, PP10 fluid, $p_\infty/p_c=0.985$, $p_\infty/p_c=0.622$
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1° source of uncertainty: thermodynamic model (3 uncertainties)
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Three parameters of Peng-Robinson equation of state

$$p = \frac{RT}{v-b} - \frac{a}{v^2 + 2bv - b^2}$$
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Freestream conditions: $M_\infty$, $\rho_\infty/\rho_c$, $\rho_\infty/\rho_c$
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- **Objective**: shape optimization for minimizing drag coefficient $C_D$

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1° source of uncertainty: thermodynamic model (3 uncertainties)

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Globally 9 uncertainties
Methodology and tools

- Full optimization
Methodology and tools

- Full optimization

Geometric DOE, 30 individuals
Methodology and tools

- Full optimization

Geometric DOE, 30 individuals
Methodology and tools

- Full optimization

Geometric DOE, 30 individuals

Uncertainty quantification: 9 uncertainties

mean($C_D$), var($C_D$)
Methodology and tools

- Full optimization

  Geometric DOE, 30 individuals

Uncertainty quantification:
9 uncertainties

\[
\text{mean}(C_D), \text{var}(C_D)
\]
Methodology and tools

- **Full optimization**

  - **Uncertainty quantification**: 9 uncertainties
  - **Geometric DOE, 30 individuals**
  - **Optimizer**: Bi-objective optimization → minimization of $\text{mean}(C_D)$ and $\text{var}(C_D)$

$\text{mean}(C_D), \text{var}(C_D)$
Methodology and tools

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Methodology and tools

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Uncertainty quantification:
- 9 uncertainties

Non-intrusive Polynomial Chaos based approach (NISP libraries):
- For 9 uncertainties and 2° order
- $19,683$ evaluations

$\text{mean}(C_D), \text{var}(C_D)$
Methodology and tools

- Full optimization

- Uncertainty quantification: 9 uncertainties

- Geometric DOE, 30 individuals

- Optimizer: Bi-objective optimization → minimization of mean($C_D$) and var($C_D$)

- mean($C_D$), var($C_D$)
Methodology and tools

- **Full optimization**

Optimizer:

- Bi-objective optimization
  - minimization of $\text{mean}(C_D)$ and $\text{var}(C_D)$

**Genetic Algorithm:**
- 30 individuals let evolve during 40 generations
- $\Rightarrow$ 1200 individuals

Optimizer:

- Bi-objective optimization $\Rightarrow$
  - minimization of $\text{mean}(C_D)$ and $\text{var}(C_D)$
Methodology and tools

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Geometric DOE, 30 individuals

Optimizer:
Bi-objective optimization → minimization of
mean($C_D$) and var($C_D$)

mean($C_D$), var($C_D$)
Methodology and tools

- **Full optimization**

  **Geometric DOE, 30 individuals**

  **Optimizer**: Bi-objective optimization → minimization of $\text{mean}(C_D)$ and $\text{var}(C_D)$

  **Global Cost**: $19683 \times 1230 = 24210090$ evaluations
  NOT FEASIBLE

  **Uncertainty quantification**: 9 uncertainties

  **mean($C_D$), var($C_D$)**
Methodology and tools

- **Approach followed: Two ways of reducing cost**
  - **Uncertainty quantification:** 9 uncertainties
  - **Geometric DOE, 30 individuals**
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Methodology and tools

- **Approach followed**: Two ways of reducing cost

- **Uncertainty quantification**: 9 uncertainties
Methodology and tools

- **Approach followed**: Two ways of reducing cost

  - **Preliminary analysis on the base airfoil** in order to reduce the number of uncertainties:
    - *Sparse Grid integration* and variance decomposition

**Uncertainty quantification**: 9 uncertainties
Methodology and tools

- Approach followed: Two ways of reducing cost

  Preliminary analysis on the base airfoil in order to reduce the number of uncertainties:
  **Sparse Grid integration and variance decomposition**

  - Reduction to 3 uncertainties

Uncertainty quantification: 9 uncertainties
Preliminary analysis of uncertainties

- Thermodynamic model (Peng-Robinson) : $c v_\infty (T_c)/R$, $\omega$, nexp
- Freestream conditions : $M_\infty$, $p_\infty /p_c$, $\rho_\infty /\rho_c$
- Geometry : three Bezier points $x1$, $x2$, $x3$
Preliminary analysis of uncertainties

- Thermodynamic model (Peng-Robinson): $c v_\infty(T_c)/R, \omega, nexp$
- Freestream conditions: $M_\infty, p_\infty/p_c, \rho_\infty/\rho_c$
- Geometry: three Bezier points $x_1, x_2, x_3$

![Graph showing distributions of $c v_\infty(T_c)/R$, $\omega$, and $nexp$. The graph displays two distributions: Gaussian and Uniforme.](image-url)
Preliminary analysis of uncertainties

- Thermodynamic model (Peng-Robinson): $c_v(\frac{T_c}{R}), \omega, \text{nexp}$
- Freestream conditions: $M_\infty, p_\infty / p_c, \rho_\infty / \rho_c$
- Geometry: three Bezier points $x_1, x_2, x_3$
Preliminary analysis of uncertainties

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- Geometry: three Bezier points $x_1, x_2, x_3$
Preliminary analysis of uncertainties

- Thermodynamic model (Peng-Robinson): $c v_\infty(T_c)/R, \omega, n_{exp}$
- Freestream conditions: $M_\infty, p_\infty/p_c, \rho_\infty/\rho_c$
- Geometry: three Bezier points x1, x2, x3

Uncertainties on the operating conditions can be considered the fundamental parameters for stochastic dense gas numerical simulation.
Methodology and tools

- Approach followed: Two ways of reducing cost
  - Geometric DOE, 30 individuals
  - Optimizer: Bi-objective optimization → minimization of mean($C_D$) and var($C_D$)

Uncertainty quantification: 9 uncertainties

mean($C_D$), var($C_D$)
Methodology and tools

- Approach followed: Two ways of reducing cost

Optimizer: Bi-objective optimization → minimization of mean($C_D$) and var($C_D$)
Methodology and tools

- Approach followed: Two ways of reducing cost

  Metamodel based approach
  - Substitute functions built by starting from the geometric DOE (by means of response surface)
  - Minimization of the substitute functions
  - Stochastic Evaluation of the best individuals

Optimizer:
Bi-objective optimization → minimization of mean($C_D$) and var($C_D$)
Methodology and tools

- **Approach followed**: Two ways of reducing cost

  - **Optimizer**: Bi-objective optimization → minimization of $\text{mean}(C_D)$ and $\text{var}(C_D)$

  - **Metamodel based approach**:
    - Substitute functions built by starting from the geometric DOE (by means of response surface)
    - Minimization of the substitute functions
    - Stochastic Evaluation of the best individuals

- **Different DOE**:
  - QuasiMonteCarlo (QMC)
  - BoxWilson
Methodology and tools

- **Approach followed**: Two ways of reducing cost

  - **Optimizer**: Bi-objective optimization → minimization of \( \text{mean}(C_D) \) and \( \text{var}(C_D) \)

  - **Metamodel based approach**
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  - **Geometric DOE**, 30 individuals
  - **Optimizer**: Bi-objective optimization → minimization of $\text{mean}(C_D)$ and $\text{var}(C_D)$
  - **Uncertainty quantification**: 9 uncertainties
  - $\text{mean}(C_D)$, $\text{var}(C_D)$
Methodology and tools

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  Geometric DOE, 30 individuals
  
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- **Optimizer**: Bi-objective optimization → minimization of \( \text{mean}(C_D) \) and \( \text{var}(C_D) \)

- **Uncertainty quantification**: 3 uncertainties

\[ \text{mean}(C_D), \text{var}(C_D) \]
Methodology and tools

- Approach followed: Two ways of reducing cost
  - Geometric DOE, 30 individuals
  - Uncertainty quantification: 3 uncertainties

\[ \text{mean}(C_D), \text{var}(C_D) \]
Methodology and tools

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- **Uncertainty quantification:** 3 uncertainties

- **Variables:** mean($C_D$), var($C_D$)
Methodology and tools

- Approach followed: Two ways of reducing cost

  Geometric DOE, 30 individuals

  Metamodel based approach → minimization of mean(C_D) and var(C_D)

Global Cost =
= Prel.An. + UQ(3) * (DOE) + Check apost.
  1000 + 27 x 30 + 27x5 = 1940 evaluations

FEASIBLE
Shape optimization

- Different strategies are compared

- Individual from the classical optimization, has a mean value lower than all the other individual of Pareto Front.

- “Uncertain” optimization allows obtaining an individual more stable (with a lower variance)
Shape optimization

Different strategies are compared

Mean solution and variance (max = 0.567) for the classical optimization

Mean solution and variance (max = 0.452) for the “uncertain” optimization
Shape optimization

- Application of previous strategy to optimize the turbine blade design and operating conditions

1° source of uncertainty: thermodynamic model

2° source of uncertainty: inlet conditions

3° source of Uncertainty: geometric tolerances

Sources of uncertainty

- Application of previous strategy to optimize the turbine blade design and operating conditions

**TD**

<table>
<thead>
<tr>
<th></th>
<th>( n )</th>
<th>( c_{\infty} )</th>
<th>( \omega )</th>
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<tbody>
<tr>
<td>Mean</td>
<td>0.5729</td>
<td>105.86</td>
<td>0.7361</td>
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<tr>
<td>Range</td>
<td>0.5385-0.6073</td>
<td>99.50-112.20</td>
<td>0.7214-0.7508</td>
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**OC + GEOM**

<table>
<thead>
<tr>
<th>( \frac{T_{in}}{T_c} )</th>
<th>( \frac{p_{in}}{p_c} )</th>
<th>( \frac{p_{out}}{p_c} )</th>
<th>( \beta )</th>
<th>( \theta )</th>
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</thead>
<tbody>
<tr>
<td>Mean</td>
<td>1.039</td>
<td>0.910</td>
<td>0.600</td>
<td>30.0</td>
</tr>
<tr>
<td>Range</td>
<td>0.9972-1.080</td>
<td>0.8736-0.9464</td>
<td>0.576-0.624</td>
<td>29.7-30.3</td>
</tr>
</tbody>
</table>

- Several output parameters to analyze Carnot efficiency, Output power, thermodynamic efficiency ...
ANOVA analysis

- Application of previous strategy to optimize the turbine blade design and operating conditions

- Three parameters are the most important
Robust Optimization

- Application of previous strategy to optimize the turbine blade design and operating conditions

- Pareto Front for mean/standard deviation of power output
Robust Optimization

- Application of previous strategy to optimize the turbine blade design and operating conditions

Nearly smooth monotonic dependence of the mean and the variance of the power output PO on the stagger angle
Conclusions & Perspectives

- Feasibility study performed for dense gas flows over an isolated airfoil → application on a realistic turbine geometry
- Full optimization → excessive computational cost
- Two ways of reducing cost
  - Stochastic evaluation by saving the most influential parameters → 3 uncertainties
  - Construction of substitute functions by starting from a DOE
- Bi-objective optimization to reduce mean and variance of the drag coefficient (3 uncertainties retained from the previous analysis) → Pareto front of optimal geometries