Development of advanced models for transition to turbulence in hypersonic flows
Prediction of transition under uncertainties
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Atmospheric reentry high speed & potential energy converted into heat

Space vehicles need heat shields (TPS)

Turbulent heat rates several times higher than in the laminar regime

Safety margins are necessary for the design of the TPS

Quantify the margins for a less conservative design

Mars Exploration Rover (MER)

MSL CFD in reentry conditions

MSL Mach 10, $\alpha = 16$-deg

Data and Comparisons from AEDC Tunnel 9

Transition prediction – The State of the Art

- **Experiments**: empirical criteria and correlation (Shuttle, Van Driest)
  - **Good**: successfully used (Apollo, Shuttle);
  - **Bad**: expensive, limited in time and no real operating conditions (Re, Ma);

- **CFD**: Transition models (Menter, Goldberg, $R-\gamma$)
  - **Good**: fast, design;
  - **Bad**: simplified physics, very sensitive to free stream conditions (Re, Ma, Tu);

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G. Serino, F. Pinna, P. Rambaud, “Numerical computations of hypersonic boundary layer roughness induced transition on a flat plate”, 2012
Three pillars for predictive engineering simulations

Transition prediction – What we propose

- Introduce **Uncertainty Quantification** (UQ) in deterministic simulations for transition prediction to:
  - Take into account the *physical variability* of the system to simulate
  - Transition is a *stochastic process*
  - *Improve* and *verify* transition tools currently used in design
  - A *stochastic model* for transition prediction does not yet exist
Outline

1. **Introduction to deterministic and probabilistic tools**
   - Linear Stability Theory and transition prediction
   - Uncertainty Quantification and numerical simulations

2. **Formulation of the method**
   - Assumptions for the deterministic simulations
   - Description of the method

3. **The VKI-H3 test case**
   - The forward problem
   - The inverse problem

4. **Conclusions & Future works**
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1. Introduction to deterministic and probabilistic tools

Linear Stability Theory and transition prediction

- Small disturbances: baseline + disturbances;
- Linearization of Navier-Stokes equations + parallel flow approximation;

\[ u = \bar{u} + u' \]
\[ \frac{\partial u'}{\partial x} + \frac{\partial v'}{\partial y} = 0 \]
\[ \frac{\partial u'}{\partial t} + \bar{u} \frac{\partial u'}{\partial x} + v' \frac{\partial \bar{u}}{\partial y} = -\frac{1}{\rho} \frac{\partial p'}{\partial x} + \nu \left[ \frac{\partial^2 u'}{\partial x^2} + \frac{\partial^2 u'}{\partial y^2} \right] \]
\[ \frac{\partial v'}{\partial t} + \bar{u} \frac{\partial v'}{\partial x} = -\frac{1}{\rho} \frac{\partial p'}{\partial y} + \nu \left[ \frac{\partial^2 v'}{\partial x^2} + \frac{\partial^2 v'}{\partial y^2} \right] \]

- Wave like disturbances;
- Space amplification theory

\[ q'(x, y, t) = \tilde{q}(y) e^{i(\alpha x - \omega t)} \]

Propagation in time (real)

Propagation in space (complex)

Degrez G., “Two dimensional boundary layer”, 2012
Linear Stability Theory and transition prediction

• Orr-Sommerfeld equations:

\[ i\alpha (\tilde{u} - c)(\tilde{v}'' - \alpha^2 \tilde{v}) - i\alpha \tilde{v}\tilde{u}'' = \frac{1}{R} \left[ \tilde{v}^{iv} - 2\alpha^2 \tilde{v}'' + \alpha^4 \tilde{v} \right] \]

• B.C.: disturbances vanish at the wall and in the far field:

\[ \tilde{v}(0) = \tilde{v}'(0) = 0 \quad \lim_{y \to \infty} \tilde{v}(y) = \lim_{y \to \infty} \tilde{v}'(y) = 0 \]

• Eigenvalue problem;

Amplification rates contour lines for Blasius velocity profile plotted in the R-\(\alpha\) plane

Neutral Stability curve: \(c_i = 0\) boundary between damped and amplified disturbances

Degrez G., “Two dimensional boundary layer”, Course Notes, 2012
Linear Stability Theory and transition prediction

- $e^N$ transition prediction method;

\[ N = \log\frac{A}{A_0} = \int_{x_0}^{x} -\alpha_i \, dx \]

N factors computed on the HIFire I reentry vehicle
Mach number = 5.28, H = 21km

- Transition: $N$-factor = $N_{exp}$
- $N = N(\text{wind tunnel, free stream parameters})$
- $N$-factor = 4-5 (WT), 13-14 (Flight);
Uncertainty quantification and numerical simulations

- **Goal**: study how physical variability of systems affects *Quantity of Interest*
- **UQ**: End-to-end study of the reliability of scientific predictions;

\[ M \in [2.5; 3.0] \]

Mean velocity divergence field

- Mean
- Standard deviation
- Shock reflection location

Iaccarino G. et al.,
“Numerical methods for uncertainty propagation in high speed flows,”
V European Conference on Computational Fluid Dynamics, 2011
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Assumptions for the deterministic simulations

- Wave-like disturbances

\[ v(x, y, z, t) = \hat{v}(y)e^{i(kx + \beta z - m\omega t)} \]

- 2D waves (\( \beta \) vanishes);
- Spatial amplification theory: \( \omega \) real, \( \alpha \) complex, wave propagation speed \( c = \omega/\alpha_r \), amplification rate in space \( -\alpha_i \);
- Transition prediction with the \( e^N \) method: VKI-H3 \( N \)-factor = 5 (Mach 6 WT);
2. Formulation of the method

Description of the method

1. Linear Stability Analysis

LST

- \( F \in [400 - 800] \text{ kHz} \)
- VESTA (Pinna 2012)

Base solution

- Free stream conditions
- B.L. profiles (CFD, SS)

\[ N \text{-factor} \]

Masutti D., *Natural and induced transition on a 7 degree half-cone at Mach 6*, 2012.
2. Formulation of the method

**Description of the method**

2. Definition of the uncertainties

- **Frequency**
  - Input uncertainty
  - Normal pdf ($\mu_F$, $\sigma_F$)

- **Propagation**
  - Monte Carlo
  - Method of transformation

- **QoI**
  - Output pdf

Example of pdf of the input parameter for the UQ analysis
2. Formulation of the method

Description of the method

3. Output

Frequency

- Input uncertainty
- Normal pdf \( \mu_F, \sigma_F \)

\[ pdf_F \]

QoI

- Output pdf

\[ pdf_N \]

Propagation

- Method of transformation

\[ \text{Transfer Function} \]

Slope of the transfer function

\[ N \text{-factor} \]
Description of the method

4. Probability of transition

\[ p_T = 1 - \int_0^{N_{\text{crit}}} pdf(N) dN = \gamma \]

- \( p_T \), probability of transition
- \( N_{\text{crit}} \), critical N-factor at the transition onset
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4. **Conclusions & Future works**
Study of natural transition on a 7° half-cone model

- Transition detected by surface measurements of the heat flux;
- Different Reynolds number conditions;

<table>
<thead>
<tr>
<th>Test case</th>
<th>$M_{\infty}$</th>
<th>$T_\infty$ [K]</th>
<th>$Re_\infty$ [1/m]</th>
<th>$T_w$ [K]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low Reynolds</td>
<td>6.0</td>
<td>60</td>
<td>$18.0 \times 10^6$</td>
<td>294</td>
</tr>
<tr>
<td>Medium Reynolds</td>
<td>6.0</td>
<td>60</td>
<td>$22.8 \times 10^6$</td>
<td>294</td>
</tr>
<tr>
<td>High Reynolds</td>
<td>6.0</td>
<td>60</td>
<td>$27.1 \times 10^6$</td>
<td>294</td>
</tr>
</tbody>
</table>

Experimental Intermittency

\[
\gamma(x) = \frac{St(x) - St_{x=x_{onset}}}{St_{x=x_{offset}} - St_{x=x_{onset}}}
\]

Masutti D., *Natural and induced transition on a 7 degree half-cone at Mach 6*, 2012.
The forward problem

- **Goal**: computation of the probability of transition caused by assumed freestream perturbation spectrum (Frequency distribution);
- **Assumption**: transition caused by perturbations in the BL upstream of the transition location;
- **Transfer function**: Linear Stability analysis to compute \( N=N(F) \);

![N-factor -Frequency relation with VESTA](image)

**Experimental transition onset**

\( N = 5 \)
3. The VKI-H3 test case

The forward problem

- **UQ approach**: free stream perturbations as *pdf* of the Frequency with *normal distributions*;

<table>
<thead>
<tr>
<th>Test case</th>
<th>$\mu_F$ [kHz]</th>
<th>$\sigma_F$ [kHz]</th>
<th>Range [kHz]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low Reynolds</td>
<td>330</td>
<td>10</td>
<td>200 ÷ 800</td>
</tr>
<tr>
<td>Medium Reynolds</td>
<td>410</td>
<td>20</td>
<td></td>
</tr>
<tr>
<td>High Reynolds</td>
<td>480</td>
<td>25</td>
<td></td>
</tr>
</tbody>
</table>

- Computation of the *probability of transition* and comparison with experiments;

UQ analysis (-) and experimental results (□) for different conditions.

Computed probability of transition
3. The VKI-H3 test case

**The inverse problem**

**Input parameters**

\[ s = (s_1, s_2, \ldots, s_d) \]

\[ s = (\mu_F, \sigma_F) \]

**Measurements**

\[ m = \gamma_{\exp} \]

**Noise**

\[ \eta \approx N(0, \sigma^2 I) \]

**FORWARD PROBLEM**

**Computational model**

\[ f(s) = N(F) \]

**Output**

\[ o = (f(s_1), \ldots, f(s_d)) \]

\[ p_T \]

**INVERSE PROBLEM**

**Computational model & Bayesian inversion**

\[ N(F) \]

**Distribution of the Input parameters**

\[ \text{pdf}_{\mu_F}, \text{pdf}_{\sigma_F} \]
3. The VKI-H3 test case

The inverse problem

- **VKI-H3 Low-Re**: MCMC to obtain the posterior pdf of the mean and the variance of the frequency distribution (Geweke’s test for convergence)

**Forward problem**
- $\mu_F = 330 \text{ kHz}$
- $\sigma_F = 10 \text{ kHz}$

**Inverse problem**
- $\mu_F = 333 \text{ kHz}$
- $\sigma_F = 11 \text{ kHz}$
3. The VKI-H3 test case

The inverse problem

- *Intermittency distribution*: VKI-Low Reynolds

Comparison of the experimental data with the probability of transition from MCMC.

- Good agreement with experimental intermittency;
- Some misalignments in the late transition zone (turbulent spots, non linear effects)
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Conclusions

• **Goal**: combination of deterministic and probabilistic tools for transition prediction in high speed flow;

• **Method**: forward problem (intermittency distribution for given conditions) and inverse problem (frequency distribution for given measurements);

• **Added value**
  • **Forward problem** – intermittency distributions resembling experimental data with fast and reliable computations (LST + e^N method);
  • **Inverse problem** – inferring perturbation spectrum for given conditions;

Future works

• **RANS model for transition prediction**: using the forward model to build a look-up table to obtain intermittency distributions at different conditions (Stanford SU2 code);

• **New stochastic transition prediction method**;

• **Comparison with experimental data**: assessment of the assumptions for the inverse problem (frequency distributions) and comparison with experimental data;
Thanks,

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3. The VKI-H3 test case

The inverse problem

- $D$ input parameters $s = (s_1, s_2, \ldots, s_D)$ through the computational model $f(s)$ to give $K$ outputs $m = (g_1(f(s_1, r)), g_2(f(s_2, r)), \ldots, g_k(f(s_k, r)))$ with $r$ auxiliary parameters $s = (r_1, r_2, \ldots, r_N)$;
- **The forward problem**: solving $m$ with given $s$ and $r$;
- **The inverse problem**: inferring $s$ given the measurements of $m$ for given $r$;
- **Parameters**: input $s = (s_1, s_2) = (\mu_F, \sigma_F)$, auxiliary $r$ (conditions for the test cases), output $m = (\gamma_1, \gamma_2, \ldots, \gamma_k)$ at $x_1, x_2, \ldots, x_k$;
- **The strategy**: given set of noisy measurements $m = m + \eta = (\gamma_1, \gamma_2, \ldots, \gamma_k)$ to seek for the input parameters $s = (\mu_F, \sigma_F)$ using the computational model $f(s)$;
- **The Bayesian inversion**:

$$p(s|m) = \frac{p(m|s) \times p(s)}{p(m)} \propto p(m|s) \times p(s)$$

- $p(s|m)$ = posterior pdf (probability of the input given the measurements)
- $p(m|s)$ = likelihood pdf (probability of the measurements given the input)
- $p(s)$ = prior pdf (information on the input parameters)
The MCMC algorithm

Input parameter

\[ s_n \in [s_{\text{LOW}}, s_{\text{UP}}] \]

Proposed step

\[ s' = s_n + \delta_n \]

Acceptance step 1

\[ s' \in [s_{\text{LOW}}, s_{\text{UP}}] \]

To compute the likelihood probability, the forward model \( f(s) \) is used.

Compute Likelihood

\[ L(s'), L(s_n) \]

Compute ratio

\[ r = \frac{L(s')}{L(s_n)} \]

Draw \( U \) from uniform distribution

\[ U \in [0,1] \]

Acceptance step 2

\[ U < \min(r, 1) \]

New state 1

\[ s_{n+1} = s_n + \delta_n = s' \]

New state 2

\[ s_{n+1} = s_n \]

After \( N \) times, the population of the input parameters is used to infer the statistical quantities. The distribution of the \( s_n \) represents the posterior density of the inverse problem.
The Bayesian inversion

Posterior Density
Probability of the inputs given the measurements
\( \text{pdf}_{\mu_F}, \text{pdf}_{\sigma_F} \)

\[
p(s \mid m) = \frac{p(m \mid s) \times p(s)}{p(m)}
\]

Likelihood \( L(s) \)
Probability of the measurements given the inputs
\( m = \gamma_{\text{exp}} \)

Prior
Probability of the measurements
NORMALIZATION CONSTANT

Prior
Probability of the inputs parameters
ASSUMED
The inverse problem

- **MCMC algorithm**: Markov Chain Monte Carlo to obtain the posterior pdf

Starting point $\mu_0, \sigma_0$

Samples within the burn-in period

Samples for the final distributions

Final distribution