NATIONAL TECHNICAL UNIVERSITY OF ATHENS (NTUA) SCHOOL OF MECHANICAL ENGINEERING LAB. OF THERMAL TURBOMACHINES PARALLEL CFD & OPTIMIZATION UNIT (PCOpt/NTUA)



Theoretical Background of the Continuous Adjoint Method in OpenFOAM, incl. Applications

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November 9, 2022, 42 slides

PCOpt/NTUA: Research Pillars, Personnel, Funding, Comp. Infrastructure



Gradient-based Shape Optimization (ShpO) in CFD





All implemented within <u>OpenFOAM v2206</u>: OpenVFOAM *"adjointOptimisationFoam"* No need for third-party software, external scripts, etc

The Adjoint Method in Optimization Algorithms

Pressure distribution and streamlines .

Used to compute the gradient of the objective function J (or constraint functions c) w.r.t. the design variables b_n , n=1,...,N, in a problem governed by PDEs (such as the Navier-Stokes eqs.) and drive a descent method towards the optimal solution or just compute Sensitivity Maps.

The Sensitivity Map is a plot of the iso-areas of the derivative of J w.r.t. the normal displacement of points on the surface to be optimized and signifies the contribution of each part of the body surface, if deformed, to the improvement in J. It helps the designer to make decisions and take actions.

a

Sensitivity map of downforce of the VW

Polo car, computed by *adjointOptimisationFoam*. <u>Red</u> : move inwards; <u>blue</u> : outwards for better traction to the ground.

> Application funded by





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Outline



<u>Part 1:</u> Understanding Continuous Adjoint using a Quasi-1D Flow Problem (Inverse Design of an Axisymmetric Duct)

<u>Part 2:</u> Extension of the Continuous Adjoint to Multi-Dimensional & Turbulent Flows –Shape Optimization (ShpO) – Capabilities of *adjointOptimisationFoam* – Industrial Applications

Part 3: Additional Capabilities of the "in-house" OpenFOAM Adjoint Solver



Part 1: The Adjoint Method – Understanding Continuous Adjoint using a Quasi-1D Flow Problem (Inverse Design of an Axisymmetric Duct)

Inverse Design of a Quasi-1D Duct – Incompressible Flow

Objective Function (min.):

$$J = \frac{1}{2} \int_0^1 \left(p(x) - p_{tar}(x) \right)^2 dx$$

Shape (Cross-Sectional Area) Parameterization:

$$S(x,b_1,b_2,b_3,b_4)\!=\!b_1+b_2x+b_3x^2+b_4x^3$$

Design/Optimization Variables:

$$b_n, n=1,2,3,4$$

State/Primal/Flow Equations (ODEs):

$$rac{d(vS)}{dx}=0$$
 $vrac{dv}{dx}+rac{dp}{dx}=0$ State/Primal/Flow Boundary Conditions:

 $v|_{x=0} = v_0$ $p|_{x=1} = p_0$





Inverse Design of a Quasi-1D Duct – Incompressible Flow

Differentiate the objective function w.r.t. b_n:

$$\frac{\delta J}{\delta b_n} = \int_0^1 \left(p(x) - p_{tar}(x) \right) \frac{\delta p}{\delta b_n} dx, \ n = 1, ..., N$$

Differentiate the flow (primal or state) equations:

$$S \frac{d}{dx} \left(\frac{\delta v}{\delta b_n} \right) + \frac{dS}{dx} \frac{\delta v}{\delta b_n} + \frac{dv}{dx} \frac{\delta S}{\delta b_n} + v \frac{d}{dx} \left(\frac{\delta S}{\delta b_n} \right) = 0 \\ \frac{\delta v}{\delta b_n} \frac{dv}{dx} + v \frac{d}{dx} \left(\frac{\delta v}{\delta b_n} \right) + \frac{d}{dx} \left(\frac{\delta p}{\delta b_n} \right) = 0$$

$$n = 1, ..., N$$

Differentiate the flow (primal or state) BCs:

$$\begin{split} & \frac{\delta v}{\delta b_n}\Big|_{x=0} = 0, \ \ \frac{\delta p}{\delta b_n}\Big|_{x=1} = 0 \\ & \underline{\text{Adjoint}} \text{ is the art of computing } \frac{\delta J}{\delta b_n} \text{ without first computing } \frac{\delta v}{\delta b_n} \text{ and } \frac{\delta p}{\delta b_n} \text{ .} \end{split}$$

 $\partial o_n \qquad \partial o_n$

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DD: Direct Differentiation (cost scales with N)



Inverse Design of a Quasi-1D Duct – Incompressible Flow

Define & differentiate the augmented objective function or Lagrangian of J:

$$L = J + \int_0^1 q \frac{d(vS)}{dx} dx + \int_0^1 u \left[v \frac{dv}{dx} + \frac{dp}{dx} \right] dx$$
$$\frac{\delta L}{\delta b_n} = \frac{\delta J}{\delta b_n} + \int_0^1 q \frac{d}{dx} \left[\frac{\delta(vS)}{\delta b_n} \right] dx + \int_0^1 u \left[\frac{\delta v}{\delta b_n} \frac{dv}{dx} + v \frac{d}{dx} \left(\frac{\delta v}{\delta b_n} \right) + \frac{d}{dx} \left(\frac{\delta p}{\delta b_n} \right) \right] dx$$

where **q** and **u** are the adjoint pressure and velocity (1D) fields. Integrate by parts:

$$\begin{split} \frac{\delta L}{\delta b_n} = & -\int_0^1 \left[-u \frac{dv}{dx} + \frac{d(vu)}{dx} + S \frac{dq}{dx} \right] \frac{\delta v}{\delta b_n} dx + \int_0^1 \left(-\frac{du}{dx} + p - p_{tar} \right) \frac{\delta p}{\delta b_n} dx \\ & -\int_0^1 v \frac{dq}{dx} \frac{\delta S}{\delta b_n} dx + \left[(vu + qS) \frac{\delta v}{\delta b_n} \right]_{x=0}^{x=1} + \left[u \frac{\delta p}{\delta b_n} \right]_{x=0}^{x=1} + \left[vq \frac{\delta S}{\delta b_n} \right]_{x=0}^{x=1} \end{split}$$



Inverse Design of a Quasi-1D Duct – Incompressible Flow

Adjoint field eqs.:

$$\frac{du}{dx} = p - p_{tar} \qquad u \frac{dv}{dx} - \frac{d(vu)}{dx} - S \frac{dq}{dx} = 0 \quad (\text{ or } v \frac{du}{dx} + S \frac{dq}{dx} = 0$$

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Adjoint BCs:

$$\left. u \right|_{x=0} = 0, \quad q |_{x=1} = - \left. \frac{v u}{S} \right|_{x=1}$$

<u>Compare</u> with the primal (flow) problem equations & boundary conditions:

$$egin{aligned} rac{d(vS)}{dx} &= 0 & vrac{dv}{dx} + rac{dp}{dx} = 0 \ v|_{x=0} &= v_0 & p|_{x=1} &= p_0 \end{aligned}$$

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Inverse Design of a Quasi-1D Duct – Incompressible Flow

Sensitivity Derivatives (SDs):

$$\frac{\delta L}{\delta b_n} = \frac{\delta J}{\delta b_n} = -\int_0^1 v \frac{dq}{dx} \frac{\delta S}{\delta b_n} dx + vq \frac{\delta S}{\delta b_n} \bigg|_{x=1} - vq \frac{\delta S}{\delta b_n} \bigg|_{x=0}, \quad n = 1, \dots, 4$$

or:

$$\begin{aligned} \frac{\delta J}{\delta b_1} &= -\int_0^1 v \frac{dq}{dx} dx + vq|_{x=1} - vq|_{x=0} \\ \frac{\delta J}{\delta b_2} &= -\int_0^1 v \frac{dq}{dx} x dx + vq|_{x=1} \\ \frac{\delta J}{\delta b_3} &= -\int_0^1 v \frac{dq}{dx} x^2 dx + vq|_{x=1} \\ \frac{\delta J}{\delta b_4} &= -\int_0^1 v \frac{dq}{dx} x^3 dx + vq|_{x=1} \end{aligned}$$
(since:
 $S(x, b_1, b_2, b_3, b_4) = b_1 + b_2 x + b_3 x^2 + b_4 x^3$)

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Optimization Methods once gradient have been computed

Steepest descent:

 $ec{b}^{k+1} = ec{b}^k - \eta \left.rac{\delta J}{\delta ec{b}}
ight|^k$

or Quasi-Newton methods (BFGS, LBFGS, DBFGS, SR1):

$$\vec{b}^{k+1} \!=\! \vec{b}^k \!+\! \Delta \vec{b}, \quad \Delta \vec{b} \!=\! -H^{-1} \frac{\delta J}{\delta \vec{b}} \qquad (H \approx \delta^2 J / \delta \vec{b}^2)$$

(for the computation of the Exact Hessian matrix see papers cited below). or the Conjugate Gradient method.

For **Constrained Optimization**: SQP and Constraint Projection.

► All available in *adjointOptimisationFOAM*.

هي International Journal for Numerical Methods in Fluids, 56(10):1929-1943, 2008. هي Computers & Fluids, 37:1029-1039, 2008. هي International Journal for Numerical Methods in Fluids, Vol. 68(6):724-739, 2012.





Inverse Design of a Quasi-1D Duct – Incompressible Flow



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From Continuous to Discrete Adjoint

$$\begin{array}{lll} \text{Minimize} & F = F(\overrightarrow{U}(\overrightarrow{b}),\overrightarrow{b}) \\\\ \text{Subject to} & \overrightarrow{R} &= \overrightarrow{R}(\overrightarrow{U}(\overrightarrow{b}),\overrightarrow{b}) &= 0 \end{array}$$

Both in discrete form





Methods/software/results in this presentation rely exclusively on <u>Continuous Adjoint</u>.



Part 2:

Extension of the Continuous Adjoint to Multi-Dimensional & Turbulent Flows for Shape Optimization (ShpO)-Capabilities of *adjointOptimisationFoam*! Industrial Applications

Continuous Adjoint in 2D/3D Laminar Flows- ShpO – Primal Eqs.

Laminar flow of an incompressible fluid :

$$\begin{split} R^p \! = \! - \! \frac{\partial v_j}{\partial x_j} \! = \! 0 \\ R^v_i \! = \! \frac{\partial (v_j v_i)}{\partial x_i} \! - \! \frac{\partial \tau_{ij}}{\partial x_j} \! + \! \frac{\partial p}{\partial x_i} \! = \! 0 , \qquad i = 1, 2(, 3) \end{split}$$
 where $\tau_{ij} \! = \! \nu \left(\frac{\partial v_i}{\partial x_j} \! + \! \frac{\partial v_j}{\partial x_i} \right)$.

For turbulent flows, see next slides.

Steps in the development of the Continuous Adjoint Method to this flow model:

- **1.** Differentiate the primal equations (PDEs) and J w.r.t. b_n.
- 2. Derive adjoint equations (field eqs. in the form of PDEs, as well as BCs).
- 3. Discretize & solve the (primal &) adjoint PDEs.
- 4. Compute grad(J), a.k.a. Sensitivity Derivatives (SDs). Ready to update b_n!



Adjoint-based Optimization (adjointOptimisationFoam)



Continuous Adjoint in 2D/3D Flows- ShpO - Total/Partial Derivatives







Partial (b_n) & spatial (x_k) derivatives permute!

$$\frac{\partial}{\partial b_n} \left(\frac{\partial \Phi}{\partial x_j} \right) = \frac{\partial}{\partial x_j} \left(\frac{\partial \Phi}{\partial b_n} \right)$$

Total (b_n) & spatial (x_k) derivatives don't!

$$\frac{\delta}{\delta b_n} \left(\frac{\partial \Phi}{\partial x_j} \right) = \frac{\partial}{\partial x_j} \left(\frac{\delta \Phi}{\delta b_n} \right) - \frac{\partial \Phi}{\partial x_k} \frac{\partial}{\partial x_j} \left(\frac{\delta x_k}{\delta b_n} \right)$$

The math. development of the adjoint method & the handling of Grid Sensitivities gives rise to 3 continuous adjoint formulations:

- Field Integral (FI) Adjoint
- Enhanced-Surface Integral (E-SI) Adjoint
- Severed SI Adjoint

The <u>FI Adjoint</u> Formulation (FI: Field Integral)

• The resulting SDs include field integrals of Grid Sensitivities $\delta x_i / \delta b_n$. An example of such a term in the SD expression is:



$$\frac{\delta J}{\delta b_{n}} = \dots + \int_{\Omega} \left\{ -u_{i}v_{j}\frac{\partial v_{i}}{\partial x_{k}} - u_{j}\frac{\partial p}{\partial x_{k}} - \tau_{ij}^{a}\frac{\partial v_{i}}{\partial x_{k}} + u_{i}\frac{\partial \tau_{ij}}{\partial x_{k}} + q\frac{\partial v_{j}}{\partial x_{k}} \right\} \frac{\partial}{\partial x_{j}} \begin{pmatrix} \delta x_{k} \\ \delta b_{n} \end{pmatrix} d\Omega$$
Grid Sensitivities

- Computing Grid Sensitivities requires a Grid Displacement Model (GDM) & its differentiation (either using finite differences, analytical differentiation, etc).
- SDs computed by the FI Adjoint are <u>accurate</u>; however, the cost of the part of the code dealing with grid sensitivities scales with N.
- Computing Sensitivity Maps using the FI Adjoint becomes prohibitively expensive, as the number of surface nodes increases.

The <u>E-SI Adjoint</u> Formulation (E-SI: Enhanced Surface Integral)

To eliminate grid sensitivities over the domain, the Enhanced-SI (E-SI) adjoint assumes a Laplacian GDM) to be introduced into the primal equations:

$$R_i^m = rac{\partial^2 m_i}{\partial x_j^2} \!=\! 0$$

New Lagrangian & new adjoint fields (m_i^α):

$$L\!=\!J\!+\!\int_{\Omega}u_{i}R_{i}^{v}d\Omega\!+\!\int_{\Omega}qR^{p}d\Omega\!+\!\int_{\Omega}m_{i}^{a}R_{i}^{m}d\Omega$$

Grid Sensitivities are eliminated by satisfying the adjoint GDM equations:

$$R_k^{m^a} = rac{\partial^2 m_k^a}{\partial x_j^2} + rac{\partial}{\partial x_j} \left\{ u_i v_j rac{\partial v_i}{\partial x_k} + u_j rac{\partial p}{\partial x_k} + au_j rac{\partial v_i}{\partial x_k} - u_i rac{\partial au_{ij}}{\partial x_k} - q rac{\partial v_j}{\partial x_k} - rac{\partial J_{\Omega'}}{\partial x_k}
ight\} = 0$$

G→ Journal of Computational Physics, 301:1-18, 2015. *G*→ Archives of Computational Methods in Engineering, 23(2): 255-299, 2016.

The <u>E-SI Adjoint</u> Formulation (E-SI: Enhanced Surface Integral)



- Practically, the E-SI adjoint is as accurate as the FI adjoint, though much cheaper!
- What if a different (than the Laplacian) GDM is used to adapt the CFD grid to the updated geometries, during the optimization? <u>The adjoint Laplace GDM can safely be used even in this case.</u>
- A <u>Severed-SI adjoint</u> is also available (by arbitrarily eliminating the effect of Grid Sensitivities), though this is <u>NOT</u> recommended.

Ger Journal of Computational Physics, 301:1-18, 2015. Ger Archives of Computational Methods in Engineering, 23(2): 255-299, 2016.

Turbulent Flows: Continuous Adjoint & Turbulence Models



Enrich the Lagrangian by including the turbulence model eq(s). and the Hamilton-Jacobi eq. for COJ computing distances from the walls (if needed). Example: Spalart-Allmaras model:

- Extra adjoint equations (adjoint to the turbulence model PDEs), new terms in the adjoint mean flow eqs. and BCs.
- Extended to models using Wall Functions by introducing the Adjoint Wall Function.
- Similar developments for the adjoint to the k- ϵ and k- ω SST turbulence models.

ACComputers & Fluids, 38:528-1538, 2009. ACJournal of Computational Physics, 229(13): 5228-5245, 2010. AC Archives of Computational Methods in Engineering, 23(2): 255-299, 2016. ACA Archives of Computational Methods in Engineering, 23(2): 255-299, 2016.

Comparison of the FI, E-SI, Severed-SI Continuous Adjoint & FD



Turbulent flow around the NACA0012 airfoil (Re=10⁶, a_{inf}=3^o) : Lift SDs computed by the FI, Severed-SI (scaled by 10 to fit into the same diagram), E-SI adjoint and FD. SDs computed w.r.t. the x (ID<23) and y (ID>23) coordinates of 24 NURBS CPs parameterizing the two airfoil sides. The adjoint to the Spalart-Allmaras turbulence model is used in all cases.

Why insisting on (Continuous) Adjoint to Turbulence Models?





Drag SDs for the 2D Ahmed body (Re=2.89x10⁶) computed using the adjoint to the Low-Re Spalart-Allmaras model. The computed sensitivity maps for drag, with or without making the frozen turbulence assumption, are quite similar if the Spalart-Allmaras model is used, but noticeably differ for the k-ω STT model. In *adjointOptimisationFoam v2206* both are available. Findings confirmed with Finite Differences, not shown here.

The Volumetric B-Splines (of NURBS) Parameterization Tool

<u>CAD-free Parameterization</u>: Using morphing techniques based, for instance, on volumetric B-Splines. The CFD grid is adapted simultaneously with the shape to be designed. Alternatively, node-based parameterization. Returning to CAD is difficult, possibly impairing the quality of the designed shapes.







Minimization of the noise perceived by the driver. A turbulence-based objective function is used, so this problem <u>cannot</u> be solved without the adjoint to the turbulence model equations. A relatively coarse grid (2.4 Mi cells) & the Volumetric B-Splines morpher (81 DoFs) were used in the adjoint optimization. A re-evaluation of the optimal solution on a fine grid (31 Mi cells) confirmed a reduction in J_N by 25%.

Ger Computers & Fluids, 122:223-232, 2015.

Application funded by

ShpO of the Defroster Nozzle of the HVAC unit of a Car



Initial

Optimized

ShpO of the defroster nozzle of the HVAC unit of a TOYOTA passenger car, for improved defrosting/ demisting performance of the windshield. The objective was to shorten the time for dispelling condensation or frost on the windshield in the most uniform way by reaching a certain air velocity close to the windshield. The optimized geometry was manufactured (3D printing) and submitted to a defrost test in the TME's climate chamber (@ -20°), leading to 15% less windshield defrost time. Green areas in the velocity isolines' plot on the windshield correspond to v^{target}.

Application funded by TOYOTA

Parallel CFD & Optimization Unit, Lab. Of Thermal Turbomachines, School of Mechanical Engineering, NTUA (PCOpt/NTUA)

Multi-Point Aerodynamic ShpO of a Concept Car

• ShpO of an ultra-lightweight vehicle, designed by the Toyota Aerodynamic Dept., for making it less sensitive to side-wind (30° from the port side; min. yaw moment), while maintaining a very low drag at 0° (longitudinal wind).

- Objective function:
- $J\!=\!\omega_D C_D^{0^o}\!+\!\omega_M C_M^{30^o}$
- <u>Pareto front</u> computed by optimizing with different values of (ω_D, ω_M) .
- Two simultaneously acting morphing boxes at the spoiler and diffuser areas.

• RANS-based adjoint optimizaton using the adjoint to the Spalart-Allmaras model (with wall functions) & a coarse polyhedral grid with ~1.6Mi cells (average y⁺=32 at the first cell-centers off the walls).



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Parallel CFD & Optimization Unit, Lab. Of Thermal Turbomachines, School of Mechanical Engineering, NTUA (PCOpt/NTUA)



Multi-Point Aerodynamic ShpO of a Concept Car



Optimized geometries (port side) compared to the BLC (starboard side). Drag reduction at 0° results from a lowered spoiler, boat-tailing and a prolonged and widened diffuser. In contrast, yaw moment reduction at 30° comes mainly from the increased spoiler height and the slight widening of the car; these increase pressure on the port side and decrease it on the starboard side to counter-balance the yaw moment of the side-wind.

& Structural and Multidisciplinary Optimization, 59(2): 675–694, 2019.



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Hydraulic Turbine Applications - Shape Optimization of a Francis Runner



Redesigning the blades for min. cavitation. To suppress cavitation, the lowest pressure on the runner surface should become greater than the vapor pressure of the fluid. Adjoint is challenging since "min." is <u>non-differentiable</u> and needs to be replaced by a (differentiable) sigmoid function.

Ser Computer Methods in Applied Mechanics and Engineering, 278:621-639, 2014.



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Part 3: Additional Capabilities of the in-house OpenFOAM Adjoint Solver

Unsteady Adjoint: Flow Fields' Storage supported by Lossless/Lossy Compression



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Unsteady Adjoint: ShpO of the Drivaer car for min. Drag



Benefits of using RPM in both Flow & Adjoint Solvers

Use of the **Recursive Projection Method (RPM)** to stabilize steady primal & adjoint solvers in case of convergence issues due to mild flow unsteadiness. The gain is that steady solvers can be used in the optimization.





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Topology Optimization (TopO), even with Conjugate Heat Transfer in Bi-Fluid Device



Example: Design of a compact bi-fluid counter-flow heat-exchanger with many inlets/outlets.

Objectives: Max. heat transfer between the cold/cold streams; also, min. total pressure losses.

<u>Constraints:</u> (1) Fluid Volumes<Threshold. (2) Equal flowrates at the 8 blue/cold exits. (3) Avoid merging the fluid streams. (4) Min. thickness of the wall separating fluid streams.

Research funded by HEAVY INDUSTRIES

TopO with CHT for the Design of a Bi-Fluid Heat Exchanger



TopO with CHT for the Design of a Bi-Fluid Heat Exchanger



TopO with CHT for the Design of a Bi-Fluid Heat Exchanger

Last step: A body-fitted grid is generated & CHT ShpO based on RANS is performed. This ends up T with less ΔP_t by 30%, while maintaining the same amount of exchanged heat.



Other Topics

- Uncertainty Quantification (UQ) based on Adjoint-Assisted Polynomial Chaos Expansion (APCE) & the Method of Moments (MoMs): First-Order Second-Moment (FOSM) & Second-Order Second-Moment (SOSM). Use of projection-based variants of FOSM & APCE, to be referred to as pFOSM & pAPCE, for gradient-based shape optimization, in the presence of uncertainties.
- Development of accurate discretization schemes for the continuous adjoint equations, inspired by (hand-differentiated) discrete adjoint.

Publicly Available Tools (in OpenFOAM):

Version	Contributions	Open VFOAM	
v1906		ressible, steady-state flows Allmaras turbulence model ivity maps	
v1912	 Surface/volume parameterization using volumetric B-Splines Automated shape optimization loop 		
v2006	New objective function	New objective function for noise minimization	
v2112	Smoothing of sensitivity maps using a Laplace-Beltrami operator		
v2206	• Adjoint to the k-ω SST turbulence model		

The latest version of the software can be downloaded from <u>https://develop.openfoam.com/Development/openfoam</u> The development branch can be found in <u>https://develop.openfoam.com/Development/openfoam/-/tree/develop</u> Extensive user-guide is available at <u>openfoam.com/documentation/files/adjointOptimisationFoamManual_v2006.pdf</u>

Coming Event!





1-3 June 2023, Chania, Crete, Greece 15th International Conference on Evolutionary and Deterministic Methods for Design, Optimization and Control

An ECCOMAS Thematic Conference

EUROGEN 2023 is the **fifteenth edition** of the **Conference on Evolutionary and Deterministic Methods for Design**, **Optimization and Control** and one of the Thematic Conferences of the <u>European Community on Computational</u> <u>Methods in Applied Sciences (ECCOMAS)</u>.

The Conference will be held at the Hotel Minoa Palace in Chania, Crete, Greece

Deadline for Abstract Submission: 5 November 2022 (but...)