Adjoints and Anisotropic Mesh Adaptation for Compressible Gas Dynamics

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San Diego, 22 Juin 2013

- History, Context and Motivations
- 2 Metric-Based Mesh Adaptation for Steady Flows
- Metric-Based Mesh Adaptation for Unsteady Flows



Early CFD (as recollected by O. Pironneau)

- 1972 Unstructured meshes introduced at Dassault by Pierre Perrier
- 1973 First FEM code runs in 3D (J. Periaux et al)
- 1976 Transonic flow as an abstract least square and use conjugate gradient
- 1977 Meeting with Antony Jameson at the von Karman Institute
- 1978 Full potential flow computation around a flacon jet
- 1983 Van Leer & Phil Roe visits INRIA-Sophia and work with Alain Dervieux
- 1987 Hermes Program



M. O. Bristeau, O. Pironneau, R. Glowinski, J. Periaux, and P. Perrier, On the numerical solution of nonlinear problems in fluid dynamics by least squares and FEM. Comput. Methods Appl. Mech. Engrg., Vol. 17/18(part 3), pp. 619-657, 1979

$\mathsf{CAD} \ \longrightarrow \ \textbf{MESH} \ \longrightarrow \ \mathsf{SOLVER} \ \longrightarrow \ \mathsf{VISU} \ / \ \mathsf{ANALYSIS}$

1 no mesh = no simulation

• a "bad" mesh implies a wrong or inaccurate solution

Automated Unstructured Tetrahedra Mesh Generation Methods:

- Octree-like [Yerry and Shephard, IJNME 1984], ...
- Advancing front [Lohner and Parikh, IJNMF 1988], [Peraire et al., IJNME 1988], [Jin and Tanner, IJNME 1991], ...
- Delaunay [Hermeline, RAIRO AN 1982], [Baker, AIAA 1987], [George, Hecht and Saltel, ICSE 1990], [Weatherhill, CMA 1992], ...
- Minimal volume [Coupez, REEF 2000], ...
- Coupled Delaunay-frontal [Marcum and Weatherhill, AIAA 1995], ...

At the end of 90's

3D powerful and mature mesh generation methods become available

 $\mathsf{CAD} \longrightarrow \mathsf{MESH} \longrightarrow \mathsf{SOLVER} \longrightarrow \mathsf{VISU} / \mathsf{ANALYSIS}$

- 1 no mesh = no simulation
- 2 a "bad" mesh implies a wrong or inaccurate solution
 - Address ever increasing geometrical complexity
 ⇒ take into account geometric features inside the mesh







1990 $h_{surf} = 10 \text{ cm}$

 $\begin{array}{l} 2000 \\ h_{surf} = 1 \ {\rm mm} \ \ {\rm and} \ \ h_{BL} = 1 \ \mu {\rm m} \end{array}$

Address ever increasing physical complexity

Anisotropic Mesh Adaptation for CFD

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- Address ever increasing physical complexity
 ⇒ take into account flow characteristics inside the mesh



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 - Address ever increasing physical complexity
 - Address convergence studies in 3D

$$\begin{array}{lll} h \rightarrow N & \text{and} & dt \sim h & \implies & \mathsf{CPU} \times \mathbf{1} \\ \\ \frac{h}{2} \sim 8N & \text{and} & dt \sim h \sim \frac{dt}{2} & \implies & \mathsf{CPU} \times \mathbf{16} \\ \\ \\ \frac{h}{4} \sim 64N & \text{and} & dt \sim h \sim \frac{dt}{4} & \implies & \mathsf{CPU} \times \mathbf{256} \end{array}$$

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Structured boundary layer mesh generation:

• Open advancing-layer method

[Lohner and Parikh, IJNMF1988], [Kallinderis and Ward, AIAA 1993], [Pirzadeh, AIAA 1994], [Marcum, AIAA 1995], [Sharov and Nakahashi, AIAAJ 1998], [Garimella and Shephard, IJNMF 2000], ...

Closed advancing-layer method by pushing

[Hassan et al, IJNME 1996], [Ito and Nakahashin, IMR 2002], [Bottasso and Detomi, 2002], ...

• Closed advancing layer method with iterative point insertion [Marcum, AIAA 1995], [Loseille and Lohner, AIAA 2011], ...

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Anisotropic Mesh Adaptation:

• Error measures with directions in 2D. Use local mapping [Peraire et al., JCP 1987], [Lohner, CMAME 1989], [Selmin and Formaggia, IJNME 1992], ...

In 1994, **O. Zienkiewicz and J. Wu.** gave a status. Even if they had great success with such approach, they said:

"Unfortunately the amount of elongation which can be used in a typical mesh generation by such mapping is small..."

 $\mathsf{CAD} \ \longrightarrow \ \mathsf{MESH} \ \longrightarrow \ \mathsf{SOLVER} \ \longrightarrow \ \mathsf{VISU} \ / \ \mathsf{ANALYSIS}$

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 \implies But, mesh anisotropy was small

- Stretched elements with a Delaunay approach in 2D [Mavriplis, JCP 1990]
- Introduce the use of metrics in a 2D Delaunay mesh generator [George, Hecht and Vallet, AES 1991]

What's a metric and metric-based mesh generation ?

I How to communicate with an automatic mesh generator ?

Main idea: change mesh generator distance and volume computation [George, Hecht and Vallet., Adv. Eng. Software 1991]

Fundamental concept: The notion of metric and Riemannian metric space

Computing geometric quantities in Riemannian metric space $\mathbf{M} = (\mathcal{M}(\mathbf{x}))_{\mathbf{x} \in \Omega}$ \updownarrow Computing geometric quantities on S





Generation of Adapted Meshes

I How to communicate with an automatic mesh generator ?

Main idea: change mesh generator distance and volume computation [George, Hecht and Vallet., Adv. Eng. Software 1991]

Fundamental concept: Generate a **unit mesh** w.r.t $(\mathcal{M}(\mathbf{x}))_{\mathbf{x}\in\Omega}$

 $\forall \mathbf{e}, \ \ell_{\mathcal{M}}(\mathbf{e}) \approx 1 \text{ and } \forall \mathcal{K}, \ |\mathcal{K}|_{\mathcal{M}} \approx \begin{cases} \sqrt{3}/4 & \text{in } 2D \\ \sqrt{2}/12 & \text{in } 3D \end{cases}$



 $\textbf{Output} \ \mathcal{H}$



Anisotropic Mesh Adaptation for CFD

Generation of Adapted Meshes

- I How to communicate with an automatic mesh generator ?
- When to measure or quantify mesh size and anisotropy ?

Use appropriate error estimates

Anisotropic Mesh Adaptation State-of-the-art:

The fruitful idea of metric was widely exploited in 2D:

[Fortin et al., ECCOMAS 1996], [Castro-Diaz et al, IJNMF 1997], [Dompierre et al., AIAA 1997], [Buscaglia and Dari, IJNME 1997], [Formaggia and Perotto, NM 2001], [Picasso, SIAMJSC 2003], ...

At the end of 90's

2D anisotropic mesh adaptation proves to be efficient in CFD

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In 1997, T. Baker wrote:

"Mesh generation in three dimensions is difficult enough task in the absence of mesh adaptation and it is only recently that satisfactory three-dimensionnal mesh generators have become available. [...] . Mesh alteration in three dimensions is therefore a rather perilous procedure that should be undertaken with care"

Anisotropic Mesh Adaptation for Steady Problems

Interpolation error based mesh adaptation

Deriving the **best mesh** to observe a given solution field W

- Generic: does not depend on the PDE and numerical scheme
- Anisotropy is easily deduced

[Tam et al., CMAME 2000], [Pain et al., CMAME 2001], [Formaggia and Perotto, NM 2001], [Picasso, SIAMJSC 2003], [Formaggia et al., ANM 2004], [Bottasso, IJNME 2004], [Li et al., CMAME 2005], [Frey and Alauzet, CMAME 2005], [Gruau and Coupez, CMAME 2005], [Huang, JCP 2005], [Compere et al., 2007], ...

Issues with feature-based anisotropic mesh adaptation for CFD

- Robustness of 3D anisotropic mesher
- Loss of anisotropy for non smooth solutions: h_{min} size in singularities
- Cannot capture small scales of the flow
- Order one convergence for non-smooth solutions with 2nd-order scheme

Anisotropic Mesh Adaptation for Steady Problems

Mesh adaptation is a non-linear problem

 \implies an iterative process is required to converge the couple mesh-solution



Anisotropic Mesh Adaptation for Steady Problems

- EPIC [Michal and Krakos, AIAA 2012]
- Feflo.a [Loseille and Lohner, AIAA 2010]
- Forge3d [Coupez, REEF 2000]
- Fun3d [Jones et al., AIAA 2006]
- MAdLib [Compere et al., IJNME 2010]
- MeshAdap [Li et al., IJNME 2005]
- Mmg3d [Dobrzynski and Frey, IMR 2008]
- Mom3d [Tam et al., CMAME 2000]
- Tango [Bottasso, IJNME 2004]
- Libadaptivity [Pain et al., CMAME 2001]

We proposed a continuous mesh framework to theorize mesh adaptation

[Alauzet et al., IMR 2006], [Alauzet, IJNMF 2008], [Loseille and Alauzet, SINUM 2010]

Discrete Element KVolume |K|Mesh \mathcal{H} of Ω_h Number of vertices N_v Linear interpolate $\prod_h u$

Continuous

Metric tensor \mathcal{M}

Volume $\alpha (\det \mathcal{M})^{-\frac{1}{2}}$

Riemannian metric space $M = (\mathcal{M}(x))_{x \in \Omega}$

Complexity
$$C(\mathbf{M}) = \int_{\Omega} \sqrt{\det(\mathcal{M}(\mathbf{x}))} d\mathbf{x}$$

Continuous linear interpolate $\pi_{\mathcal{M}} u$

Local interpolation error duality

For all *K* unit for *M* and for all *u* quadratic positive form $(u(\mathbf{x}) = \frac{1}{2} {}^{t} \mathbf{x} H_{u} \mathbf{x})$: $\|u - \prod_{h} u\|_{L^{1}(K)} = \frac{\sqrt{2}}{240} \underbrace{\det(\mathcal{M}^{-\frac{1}{2}})}_{mapping} \underbrace{\operatorname{trace}(\mathcal{M}^{-\frac{1}{2}} H_{u} \mathcal{M}^{-\frac{1}{2}})}_{anisotropic term} = \|u - \pi_{\mathcal{M}} u\|_{L^{1}(K)}$

Working in this framework enables us to use powerful mathematical tool

Application: Minimizing the Interpolation Error in L^{p} -norm

• An ill-posed discrete problem

Find \mathcal{H}_{opt} having N vertices such that $\mathcal{H}_{opt}(u) = \operatorname{Arg\,min}_{\mathcal{H}} \|u - \prod_{h} u\|_{\mathcal{H}, L^{p}(\Omega_{h})}$

• A well-posed continuous problem

Find $\mathbf{M}_{L^p} = (\mathcal{M}_{L^p}(\mathbf{x}))_{\mathbf{x} \in \Omega}$ of complexity N such that

$$E_{L^{p}}(\mathbf{M}_{L^{p}}) = \min_{\mathbf{M}} E_{L^{p}}(\mathbf{M}) = \min_{\mathbf{M}} \|u - \pi_{\mathcal{M}} u\|_{L^{p}(\Omega)}$$
$$= \min_{\mathbf{M}} \left(\int_{\Omega} |u(\mathbf{x}) - \pi_{\mathcal{M}} u(\mathbf{x})|^{p} d\mathbf{x} \right)^{\frac{1}{p}}$$

 \Longrightarrow Solved by a calculus of variations

Optimal metric [Alauzet et al., IMR 2006], [Loseille and Alauzet, SINUM 2010]

$$\mathcal{M}_{L^{p}}(\mathbf{x}) = N^{\frac{2}{3}} \left(\int_{\Omega} (\det |H_{u}|)^{\frac{p}{2p+3}} \right)^{-\frac{2}{3}} (\det |H_{u}(\mathbf{x})|)^{\frac{-1}{2p+3}} |H_{u}(\mathbf{x})|$$
1

- **M**_{L^p} is unique
- M_{L^p} has for optimal directions and ratios the Hessian ones
- M_{L^p}(u) provides an optimal explicit bound of the interpolation error in L^p norm:

$$\|u - \pi_{\mathcal{M}_{L^{p}}} u\|_{L^{p}(\Omega)} = 3 N^{-\frac{2}{3}} \left(\int_{\Omega} (\det |H_{u}|)^{\frac{p}{2p+3}} \right)^{\frac{2p+3}{3p}}$$

 Global second order of convergence for a sequence of embedded continuous meshes (M^N_{L^p}(u))_{N=1...∞}

Multi-scale function

Asymptotic 2nd order cv

Feature-based Anisotropic Mesh Adaptation

We propose a multiscale anisotropic mesh adaptation

[Loseille et al., AIAA 2007], [Alauzet, IJNMF 2008], [Loseille and Alauzet, IMR 2009]

- Optimal control of the interpolation error in L^p norm : $\|W \prod_h W\|_{L^p(\Omega_h)}$
- Highly anisotropic meshes
- Capture all scales of the flow
- Global 2nd of mesh convergence for the mesh adaptation process
- Early capturing property: asymptotic convergence is reached faster

Goal-Oriented Anisotropic Mesh Adaptation

Functional approximation error based mesh adaptation

Deriving the **best mesh** to observe a given functional:

J(W) = (g, W) with $\nabla \cdot \mathcal{F}(W) = 0$

- Depends explicitely on the PDE and numerical scheme
- The goal is to derive the best solution of a PDE

[Venditti and Darmofal, JCP 2003], [Jones et al., AIAA 2006], [Power et al., CMA 2006], [Wintzer et al., AIAA 2008], [Leicht and Hartmann, JCP 2010], ...

Issues with goal-oriented anisotropic mesh adaptation

- Anisotropy is hard to prescribe
- Error estimate are difficult to obtain and are not generic:
 - Explicit use of the PDE
 - Strong dependency on the numerical scheme
- There is an over cost as it requires to compute the adjoint state

Goal-Oriented Anisotropic Mesh Adaptation

We propose a goal-oriented anisotropic mesh adaptation

[Loseille et al., AIAA 2010], [Loseille et al., JCP 2010]

• Optimal control of the approximation error in L^1 norm

 $\|J(W) - J(W_h)\|_{L^1(\Omega_h)} \approx \|\nabla W^* \cdot (\mathcal{F}(W) - \Pi_h \mathcal{F}(W))\|_{L^1(\Omega_h)}$

- Highly anisotropic meshes and capture all scales of the flow
- Global 2nd of mesh convergence for the output functional

Anisotropic Mesh Adaptation for CFD

Wing Tip Vortices Accurate Computation

Computation of wing tip vortices of a Dassault Falcon Jet:

• Adjoint functional :

$$J(W) = \int_{\gamma} \|
abla \wedge (\mathbf{u} - \mathbf{u}_{\infty}) \|_2^2 \, \mathrm{d} \gamma$$

• Adaptation variable : Mach number

Comparison between adjoint (top) and feature (bottom) based adapted meshes

Comparison between adjoint (top) and feature (bottom) based wing tip vortices

Sensitivity of Functionals of Euler Equations with Shocks

Let time-dependent function

$$J = \frac{1}{2} \int_{S \times (0,T)} |B \cdot W - b|^2 \quad \text{with} \quad \partial_t W + \nabla \cdot F(W) = 0$$

The extended calculus of variation on J gives [Alauzet and Pironneau, IJNMF 2012]

$$\delta J = \int_{S \times (0,T)} (B \cdot \overline{W} - b) B \cdot \delta W \text{ with } \overline{W} = \frac{1}{2} (W^+ + W^-)$$

Turning to δW in state equation:

$$\partial_t \delta W + \nabla \cdot (\overline{F'(W)} \delta W) = 0 \text{ and } \delta W(0) = 0$$

The adjoint equation:

$$\partial_t W^* + \overline{F'(W)} \nabla W^* = 0, \ W^*(T) = 0 \ \Rightarrow \ \int_{\partial\Omega \times (0,T)} W^* \cdot (n \cdot (\overline{F'(W)} \delta W)) = 0$$

Thus, this gives a method to evaluate continuous W^* and δJ

$$W^* \cdot (n \cdot (\overline{F'(W)})|_{\Omega} = (B\overline{W} - b)B^T \Rightarrow \delta J = -\int_{\partial \Omega \setminus S \times (0,T)} W^* \cdot (n \cdot (\overline{F'(W)} \delta W))$$

Sensitivity of Functionals of Euler Equations with Shocks

Validation on a NACA0012 airfoil that for non-smooth flow discrete adjoint converge to continuous one

The theory on the continuous systems tells that the adjoint is continuous across the shocks but maybe discontinuous elsewhere, including where W has slip-discontinuities

Sensitivity of Functionals of Euler Equations with Shocks

Validation on a NACA0012 airfoil that for non-smooth flow discrete adjoint converge to continuous one

Comparison between $(\rho v)^*$ and $(\rho_h v_h)^*$ on the observation surface S

Conclusion: discrete and continuous calculus of variation agree

Anisotropic Mesh Adaptation for CFD

Anisotropic Mesh Adaptation for Unsteady Problems

Time-accurate anisotropic mesh adaptation

Deriving the **best space-time mesh** to observe a given functional $J(W(\mathbf{x}, t)) \quad \text{with} \quad \partial_t W(\mathbf{x}, t) + \nabla \cdot \mathcal{F}(W(\mathbf{x}, t)) = 0$

[Lohner and Baum, IJNMF 1992], [De Sampaio et al., CMAME 1993], [Speares and Berzins, IJNMF 1997], [Pain et al., CMAME 2001], [Remacle et al., IJNME 2005], ...

Issues with time-accurate anisotropic mesh adaptation

- Solution evolves in time
 - Temporal error occurs
 - The mesh is always lagging behind the solution
- Steady case is applied frequently in time: each nth iterations
 - A lot of solution interpolation \implies spoil solution accuracy
 - A lot of remeshing \implies CPU cost increase
 - Require a flow solver with dynamic data
- 4D space-time anisotropic mesh adaptation

Anisotropic Mesh Adaptation for Unsteady Problems

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[Lohner and Baum, IJNMF 1992], [De Sampaio et al., CMAME 1993], [Speares and Berzins, IJNMF 1997], [Pain et al., CMAME 2001], [Remacle et al., IJNME 2005], ...

We propose a fixed-point anisotropic mesh adaptation strategy based on [Alauzet et al., IMR 2011], [Belme et al., JCP 2012]

• Optimal control of the space-time approximation error on J in L^1 norm

 $\|J(W)-J(W_h)\|_{L^1([0,T]\times\Omega_h)}\approx \|W_t^*(W-\Pi_hW)+\nabla W^*\cdot(\mathcal{F}(W)-\Pi_h\mathcal{F}(W))\|_{L^1([0,T]\times\Omega_h)}$

- Global fixed-point mesh adaptation algorithm
- Conservative solution transfer

G-O EE for Unsteady Compressible Euler Equations

Solve this problem in the continuous mesh framework

From [Loseille and Alauzet, SINUM 2010], after discarding BT:

$$\begin{split} \mathbf{E}(\mathbf{M}) &= \int_0^T \int_{\Omega} |W_t^*| |W - \pi_{\mathcal{M}} W| \, \mathrm{d}\Omega \, \mathrm{d}t + \int_0^T \int_{\Omega} |\nabla W^*| \, . \, |\mathcal{F}(W) - \pi_{\mathcal{M}} \mathcal{F}(W)| \, \mathrm{d}\Omega \, \mathrm{d}t \\ &= \int_0^T \int_{\Omega} \operatorname{trace} \left(\mathcal{M}^{-\frac{1}{2}} \, \mathbf{H} \, \mathcal{M}^{-\frac{1}{2}} \right) \, \mathrm{d}\Omega \, \mathrm{d}t \\ &\text{with} \quad \mathbf{H} = \sum_{i=1}^5 \left(|W_{i,t}^*| \, |\mathcal{H}(W_i)| + \sum_{j=1}^3 |\nabla_{x_j} W_i^*| \, |\mathcal{H}(\mathcal{F}_{x_j}(W_i))| \right) \end{split}$$

Mesh Optimization Problem

Find $\mathbf{M}_{go} = (\mathcal{M}_{go}(\mathbf{x}))_{\mathbf{x} \in \Omega}$ of complexity N_{st} such that

$$\mathbf{E}_{go}(\mathbf{M}_{go}) = \min_{\mathbf{M}} \int_{0}^{T} \int_{\Omega} \operatorname{trace} \left(\mathcal{M}^{-\frac{1}{2}} \mathbf{H} \mathcal{M}^{-\frac{1}{2}} \right) d\Omega dt$$

under constraint $C_{st}(\mathbf{M}) = N_{st} = \int_{0}^{T} \tau(t)^{-1} \left(\int_{\Omega} d_{\mathcal{M}}(\mathbf{x}, t) d\mathbf{x} \right) dt$

G-O EE for Unsteady Compressible Euler Equations

Solve this problem in the continuous mesh framework

Two steps resolution:

- 1. Spatial minimization for fixed t
- 2. Temporal minimization

Spatial minimization for fixed t

$$\mathcal{M}_{go}(\mathbf{x},t) = N(t)^{\frac{2}{3}} \mathcal{K}(t)^{-\frac{2}{3}} \left(\det \mathbf{H}(\mathbf{x},t)\right)^{-\frac{1}{5}} \mathbf{H}(\mathbf{x},t)$$

Temporal minimization for specified au [Belme et al., JCP 2012]

$$\mathcal{M}_{go}(\mathbf{x},t) = N_{st}^{\frac{2}{3}} \left(\int_0^T \tau(t)^{-\frac{2}{5}} \mathcal{K}(t) \mathrm{d}t \right)^{-\frac{2}{3}} \tau(t)^{\frac{2}{5}} (\det \mathbf{H}(\mathbf{x},t))^{-\frac{1}{5}} \mathbf{H}(\mathbf{x},t)$$

with
$$\mathcal{K}(t) = \left(\int_{\Omega} (\det \mathbf{H}(\bar{\mathbf{x}}, t))^{\frac{1}{5}} \mathrm{d}\bar{\mathbf{x}}\right)$$

Remark: A temporal minimization for time sub-intervals has also been achieved

Discrete Unsteady Adjoint Resolution

Forward in time state equation:

$$W_h^n = W_h^{n-1} + \delta t^n \Phi_h(W_h^{n-1})$$

Consider a time-dependent functional:

$$J(W) = \int_0^T \int_{\Gamma} j_{\Gamma}(W(\mathbf{x}, t)) \mathrm{d}\mathbf{x} \mathrm{d}t$$

Backward in time adjoint equation:

$$W_h^{*,n-1} = W_h^{*,n} + \delta t^n \frac{\partial J_h^{n-1}}{\partial W_h^{n-1}} (W_h^{n-1}) - \delta t^n (W_h^{*,n})^T \frac{\partial \Phi}{\partial W_h^{n-1}} (W_h^{n-1})$$

Solve state foreward: $\Psi(W) = 0$

Solve adjoint state backward: $\Psi^*(W, W^*) = 0$

Discrete Unsteady Adjoint Resolution

Problematics

 Computing W^{*,n-1} at time tⁿ⁻¹ requires the knowledge of state Wⁿ⁻¹ and adjoint state W^{*,n}

⇒ The knowledge of all states $\{W^n\}_{n=1,N}$ is needed ⇒ Large memory storage effort in 3D (10⁶ vertices & 10³ iterations request 37.25 Gb)

Reduce the memory storage effort by:

- out-of-core storage of checkpoints
 - \implies recomputing effort of the state W
- state interpolation between two memory storage
 - \implies slight loss of accuracy

Solve state once to get checkpoints $\Psi(W) = 0$

A Movie to Illustrate the Approach

High-Fidelity Blast Computation

Application: High-Resolution Blast Wave Prediction

Goal-oriented time-accurate aniso. mesh adaptation on pressure impulse

- From 40K to 1million vertices
- From 200K to 6 million tets

The observation Γ is this building

- Mean aniso ratio ≈ 100
- Mean aniso quotient ≈ 3000

High-Fidelity Blast Computation

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Conclusion

Last Decades:

- 1990's Automated 3D unstructured mesh generation \implies inviscid computation on complex geometries
- 2000's Automated 3D BL mesh generation \implies viscous computation on complex geometries
- 2010's Automated highly anisotropic mesh adaptation \implies High-fidelity inviscid computation on complex geometries

Current and Next Decades:

- Highly anisotropic mesh adaptation for viscous flows
 ⇒ Coupling structured and unstructured mesh adaptation
- Highly anisotropic mesh adaptation for very-high order solvers
 Curved meshes, very-high order error estimates
- Highly anisotropic mesh adaptation for moving geometries problem
 Adaptive moving mesh methods, dynamic error estimates

Thank you for your attention

