AEROASTRO

Four-dimensional anisotropic mesh adaptation for spacetime numerical simulations

Philip Claude Caplan

Thesis committee: Prof. David L. Darmofal (chair), Bob Haimes, Prof. Jaime Peraire

PhD Thesis Defense

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Introduction



Introduction

Mesh adaptation algorithm

Demonstration with analytic metrics Demonstration within adaptive framework

Conclusions

We want accurate answers to PDEs using numerical simulations.





783% error in drag

We want accurate answers to PDEs using numerical simulations.







783% error in drag

0.5% error in drag

"The number of wings designed and wind tunnel tested has steadily decreased." [Johnson, 2005]

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"The number of wings designed and wind tunnel tested has steadily decreased." [Johnson, 2005]



Mesh adaptation is useful for obtaining accurate solutions.





Mesh adaptation is useful for obtaining accurate solutions.





How to solve problems with time-dependent features?



[Song, 2014]

































Spacetime uniform refinement requires $\mathcal{O}(\delta^{-2})$ elements.





Spacetime tensor-product approach requires $\mathcal{O}(\delta^{-1})$ elements.



[Bangerth, 1999] [Hartmann, 2001]



Spacetime unstructured approach requires $\mathcal{O}(1)$ elements.





Spacetime unstructured approach demonstrated in 1d + t and 2d + t.





[Jayasinghe, 2018]





Introduction

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Spacetime unstructured approach demonstrated in 1d + t and 2d + t.



[Yano, 2012]



[Jayasinghe, 2018]



We need unstructured anisotropic 4*d* meshes for unsteady 3*d* problems.

Introduction

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Anisotropic meshes can be obtained using a metric field.



Optimize mesh?



Anisotropic meshes can be obtained using a metric field.



Optimize mesh?



$$\mathcal{M}^* = \operatorname*{arg\,min}_{\mathcal{M}} \underbrace{\mathcal{E}(\mathcal{M})}_{\text{error}} \quad \text{such that} \quad \underbrace{\mathcal{C}(\mathcal{M})}_{\text{cost}} \leq c_t$$

Optimize metric field? [Loseille, 2011]



Anisotropic meshes can be obtained from a metric-conforming mesher.





Anisotropic meshes can be obtained from a metric-conforming mesher.





Anisotropic meshes can be obtained from a metric-conforming mesher.





Introduction

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Previous attempts at anisotropic 4d meshing were not successful.



[Coupez, 2000] & [Gruau, 2005]

- Star operator for local mesh operations,
- Minimum volume principle,
- Uniform metric fields.

h	time (s)	# vertices	# elements
1/2	4	126	946
1/3	41	451	4573
1/4	179	1192	14887
1/5	547	2588	35894

[Tremblay, 2007]

- Simulated edge swapping,
- Poor metric-conformity (aspect ratio 10:1),
- Heat equation in 3d+t with isotropic meshes.



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Thesis objectives & contributions



Main objective:

Develop an anisotropic four-dimensional meshing capability for adaptive numerical simulations.

Approach:

- Simplex meshes (triangles, tetrahedra, pentatopes).
- Local cavity operator framework.
- Mesh Optimization via Error Sampling and Synthesis.

Contributions:

- (1) Develop an <u>algorithm</u> and <u>software</u> for 4d metric-conforming mesh adaptation.
- (2) Validate the adaptive algorithm on 4*d* problems.
- (3) Demonstrate first PDE-driven anisotropic unstructured adaptation for unsteady 3d problems.

Four-dimensional anisotropic mesh adaptation algorithm



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Metric-conforming mesher strives to create unit *n*-simplices.



- Goals for a mesh $\mathcal{M} = (\mathcal{V}, \mathcal{T})$ of $\Omega \subset \mathbb{R}^n$
 - Edge lengths are 1:

 $\ell_{\mathbf{m}}(e) = 1, \ \forall e \in \mathcal{E}(\mathcal{T})$

• <u>Quality</u> is that of equilateral simplex:

$$q_{\mathbf{m}}(\kappa) = \frac{1}{q_{\Delta}} \frac{v_{\mathbf{m}}^{2/n}(\kappa)}{\sum\limits_{\boldsymbol{e} \in \mathcal{E}(\kappa)} \ell_{\mathbf{m}}^{2}(\boldsymbol{e})} = 1, \ \forall \kappa \in \mathcal{T}$$

• <u># simplices</u> matches metric field complexity:

$$n_{s}v_{\Delta} = \int_{\mathcal{M}} \sqrt{\det \mathbf{m}} \, \mathrm{d}\mathbf{x}$$



Metric-conforming mesher strives to create unit *n*-simplices.



Goals for a mesh $\mathcal{M} = (\mathcal{V}, \mathcal{T})$ of $\Omega \subset \mathbb{R}^n$

• Edge lengths are close to 1:

 $1/\sqrt{2} \leq \ell_{\mathbf{m}}(e) \leq \sqrt{2}, \ \forall e \in \mathcal{E}(\mathcal{T})$

• <u>Quality</u> is close to that of equilateral simplex:

$$q_{\mathbf{m}}(\boldsymbol{\kappa}) = \frac{1}{q_{\Delta}} \frac{v_{\mathbf{m}}^{2/n}(\boldsymbol{\kappa})}{\sum\limits_{\boldsymbol{e} \in \mathcal{E}(\boldsymbol{\kappa})} \ell_{\mathbf{m}}^{2}(\boldsymbol{e})} \in [0.8, 1], \ \forall \boldsymbol{\kappa} \in \mathcal{T}$$

• <u># simplices</u> matches metric field complexity:

$$n_{s}v_{\Delta} \approx \int_{\mathcal{M}} \sqrt{\det \mathbf{m}} \, \mathrm{d}\mathbf{x}$$



Local operators modify an existing mesh to meet target criteria.



Local operators modify an existing mesh to meet target criteria.



Split
Local operators modify an existing mesh to meet target criteria.





Collapse



Local operators modify an existing mesh to meet target criteria.





Collapse



Local operators modify an existing mesh to meet target criteria.







Application of mesh modification operator:

[Coupez, 2000],[Loseille, 2017]

$$\mathcal{T}^{k+1} = \mathcal{T}^k \setminus \underbrace{\mathcal{C}(f)}_{\text{cavity}} \cup \underbrace{\mathcal{B}(p, \partial \mathcal{C}^k)}_{\text{insertion}}$$





Application of mesh modification operator:

[Coupez, 2000],[Loseille, 2017]



 $\mathcal{T}^{k+1} = \mathcal{T}^k \setminus \underbrace{\mathcal{C}(f)}_{} \cup \underbrace{\mathcal{B}(p, \partial \mathcal{C}^k)}_{}$ cavity

insertion



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adaptMesh

input: $\mathcal{M}_{in} = (\mathcal{V}_{in}, \mathcal{T}_{in}), \mathbf{m}$ output: \mathcal{M}_{out} (modified)

```
\label{eq:main_stage} \begin{split} & \rhd \text{ stage 1: target edges longer than 2} \\ & \mathcal{M} \leftarrow \text{ collapseEdges}(\mathcal{M}, \textbf{m}) \\ & \mathcal{M} \leftarrow \text{ splitEdges}(\mathcal{M}, \textbf{m}, 2) \\ & \mathcal{M} \leftarrow \text{ swapEdges}(\mathcal{M}, \textbf{m}) \\ & \mathcal{M} \leftarrow \text{ smoothVertices}(\mathcal{M}, \textbf{m}) \end{split}
```



Operator schedule progressively tries to improve metric conformity.



adaptMesh

input: $\mathcal{M}_{in} = (\mathcal{V}_{in}, \mathcal{T}_{in}), \mathbf{m}$ output: \mathcal{M}_{out} (modified)

$$\begin{split} & \succ \text{ stage 2: target edges longer than } \sqrt{2} \\ & \mathcal{M} \leftarrow \text{ collapseEdges}(\mathcal{M}, \textbf{m}) \\ & \mathcal{M} \leftarrow \text{ splitEdges}(\mathcal{M}, \textbf{m}, \sqrt{2}) \\ & \mathcal{M} \leftarrow \text{ swapEdges}(\mathcal{M}, \textbf{m}) \\ & \mathcal{M} \leftarrow \text{ smoothVertices}(\mathcal{M}, \textbf{m}) \end{split}$$





adaptMesh

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Highlights:

- do not create short edges during splits
- check number of pentatopes matches metric volume in 4*d*

Demonstration with analytic metrics



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The meshing algorithm performs well on 3*d* benchmark cases.



Benchmarks of the Unstructured Grid Adaptation Working Group (UGAWG) [Ibanez et al., 2017]:



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Benchmarks of the Unstructured Grid Adaptation Working Group (UGAWG) [Ibanez et al., 2017]:





Demonstration with analytic metrics

Assessment of metric-conformity.





Length and quality histograms will be plotted on logarithmic scales.





Demonstration with analytic metrics

Length and quality histograms will be plotted on logarithmic scales.





Expect 39k tetrahedra for the Cube Linear case.





	%ℓ _{unit}	%q _{unit}	# simplices
avro	99.10 %	92.15 %	38.30k
feflo.a	98.28 %	74.28 %	45.16k
EPIC-ICSM	93.04 %	59.52 %	47.55k
Omega_h	93.00 %	47.15 %	51.67k

Expect 31.7k tetrahedra for the Cube-Cylinder Linear case.





	%ℓ _{unit}	%q _{unit}	<pre># simplices</pre>
avro	98.79 %	90.88 %	30.45k
feflo.a	93.73 %	55.65 %	46.29k
EPIC-ICSM	92.07 %	56.71 %	38.30k
Omega_h	92.79 %	47.30 %	40.96k

Expect 36.4k tetrahedra for the Cube-Cylinder Polar 2 case.





	%ℓ _{unit}	%q _{unit}	# simplices
avro	95.76 %	78.76 %	34.20k
feflo.a	93.83 %	55.92 %	53.12k
EPIC-ICSM	91.77 %	58.52 %	44.28k
Omega_h	92.19 %	44.96 %	49.15k

Let's look at some 4*d* metric-conforming cases in a tesseract.



Tesseract Linear

$$\mathbf{m}(\mathbf{x}) = \text{diag}\left(h_x^{-2}, h_y^{-2}, h_z^{-2}, h_t^{-2}\right)$$

 $h_x = h_y = h_z = h = \text{constant}$ h_t increases away from t = 0.5.

TL1 (*h* = 0.25) **TL2** (*h* = 0.125)



Tesseract Wave

$$\mathbf{m}(\mathbf{x}) = \mathbf{Q} \operatorname{diag} \left(h_r^{-2}, h_\theta^{-2}, h_\phi^{-2}, h_t^{-2} \right) \mathbf{Q}^t$$

Wave radius increases at $R(t) = R_0 + v_w t$ h_r increases away from R(t), h_t = constant h_{ϕ} , h_{θ} similar to Cube-Cylinder Polar 2 case



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Refine hyperplanes at non-constant t.

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Tesseract Wave

$$\mathbf{m}(\mathbf{x}) = \mathbf{Q} \operatorname{diag} \left(h_r^{-2}, h_{\theta}^{-2}, h_{\phi}^{-2}, h_t^{-2} \right) \mathbf{Q}^t$$

Wave radius increases at $R(t) = R_0 + v_w t$ h_r increases away from R(t), h_t = constant h_{ϕ} , h_{θ} similar to Cube-Cylinder Polar 2 case



Refine spheres at constant *t* and cones at non-constant *t*.





Demonstration with analytic metrics

















Demonstration with analytic metrics

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Expected hyperplanes are refined for the Tesseract Linear cases.





Demonstration with analytic metrics

Expected spheres and cones are refined for the Tesseract Wave case.





Good metric-conformity is observed for the 4d benchmark cases.





	%ℓ _{unit}	%q _{unit}	<pre># simplices</pre>	expected
Linear 1	96.46 %	56.35 %	55.66k	51k
Linear 2	97.27 %	70.00 %	814.50k	818k
Wave	88.96 %	26.89 %	347.19k	n/a

Demonstration within adaptive framework



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Metric fields obtained from MOESS [Yano, 2012].





Metric fields obtained from MOESS [Yano, 2012].





Metric fields obtained from MOESS [Yano, 2012].






Mesh Optimization via Error Sampling and Synthesis



Original



Mesh Optimization via Error Sampling and Synthesis



Original $\mathbf{m}_0 \quad \eta_0$



Mesh Optimization via Error Sampling and Synthesis





Mesh Optimization via Error Sampling and Synthesis



 $\begin{array}{lll} \mbox{Original} & \mbox{m}_0 & \eta_0 \\ \mbox{Edge split 1} \end{array}$



Mesh Optimization via Error Sampling and Synthesis



Original	\mathbf{m}_0	η_0
Edge split 1	\mathbf{m}_1	η_1



Mesh Optimization via Error Sampling and Synthesis



Original	\mathbf{m}_0	η_0
Edge split 1	\mathbf{m}_1	η_1
Edge split 2	\mathbf{m}_2	η_2



Mesh Optimization via Error Sampling and Synthesis



Original	\mathbf{m}_0	η_0
Edge split 1	\mathbf{m}_1	η_1
Edge split 2	\mathbf{m}_2	η_2
Edge split 3	\mathbf{m}_3	η_3



Mesh Optimization via Error Sampling and Synthesis



Original	\mathbf{m}_0	η_0
Edge split 1	\mathbf{m}_1	η_1
Edge split 2	\mathbf{m}_2	η_2
Edge split 3	\mathbf{m}_3	η_3

Error model: $\eta(\mathbf{s}) = \eta_0 \exp(tr(\mathbf{r} \mathbf{s}))$





Adapt to the exact L^2 error of a boundary layer function.





L^2 error control for boundary layer: DOF overshoot $\approx 35\%$.





p = 1 512k DOF optimized meshes show expected refinement.





p = 2 512k DOF optimized meshes show expected refinement.





Demonstration within adaptive framework

Analytic mesh distributions achieved.





Analytic mesh distributions achieved.





Adapt to the exact L^2 error of a spherical wave function.



$$u(\mathbf{x}, t) = \exp(-t) \exp\left(-200(R(t) - ||\mathbf{x}||)^2\right)$$
 with $R(t) = 0.4 + 0.7t$





DOF overshoot complemented by slight rise in error.





DOF overshoot complemented by slight rise in error.





p = 1 512k DOF optimized meshes show expected refinement.





p = 2 512k DOF optimized meshes show expected refinement.





Demonstration within adaptive framework

Metric conformity is good.





		$\%\ell_{unit}$	%q _{unit}	# simplices	% overshoot
Ì	p = 1, 64k	97.72 %	53.31 %	14.83k	15.84 %
	p = 1, 512k	97.57 %	51.76 %	116.86k	14.12 %
Ì	p = 2, 64k	98.71 %	50.15 %	4.87k	14.12 %
	p = 2, 512k	97.40 %	49.63 %	39.76k	16.47 %

Large aspect ratios are obtained.





p = 1, 512k DOF



Order / DOF	64k	128k	256k	512k
p = 1	2.07e+02	5.07e+02	8.32e+02	2.12e+03
p = 2	6.53e+01	1.26e+02	2.60e+02	5.88e+02

Unsteady advection-diffusion with a boundary layer.





Unsteady advection-diffusion with a boundary layer.





DOF overshoot as high as 43%.





p = 2 512k DOF optimized meshes show expected refinement.





Unsteady advection-diffusion with an expanding spherical wave.





Unsteady advection-diffusion with an expanding spherical wave.





DOF overshoot as high as 38%.





p = 1 512k DOF optimized meshes show expected refinement.





Demonstration within adaptive framework

Need more DOF to fully refine solution.





Spherical wave at t = 1 is captured.





Conclusions



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Summary



Main objective:

Develop an anisotropic four-dimensional meshing capability for adaptive numerical simulations.

Contributions:

- (1) Develop an <u>algorithm</u> and <u>software</u> for 4d metric-conforming mesh adaptation.
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metric-conforming

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Future work

- Parallelization of the mesh adaptation algorithm,
- Adaptation of curvilinear meshes,
- Applications of the framework to other PDEs,
- Investigating continuous Galerkin discretization,
- Mesh adaptation for higher-dimensional parameter spaces.







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Ryan & Alex





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Questions?



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Why the giraffe?





Why the giraffe?





Why the $\sqrt{2}$?



[Frey and George, 2008]: The coefficient $\sqrt{2}$ is related to the fact that an edge can be split if the lengths of the two sub-edges minimize the error distance to the unit length as compared with the initial length.

In other words:

• We want to minimize ℓ_{split} :

$$\ell_{\text{split}} = \underset{\alpha}{\operatorname{arg\,min}} \ \alpha \quad \text{such that } g(\alpha) = 2\left(\frac{\alpha}{2} - 1\right)^2 - (\alpha - 1)^2 \le 0$$

Applying the KKT conditions leads to $g(\alpha) = 0 \rightarrow \ell_{\text{split}} = \sqrt{2}$.

• We want to maximize ℓ_{collapse} but if we make it too big, then we will cycle between splitting and collapsing because splitting can create edges with length $\ell_{\text{split}}/2$. We can avoid this by setting $\ell_{\text{collapse}} = \sqrt{2}/2$.

Study of mesh adaptation components



Conclusions

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Property	Current	Variant 1	Variant 2	Variant 3	Variant 4	Variant 5
		Same Length	No Swapout	No Limit	No Smoothing	Single Stage
$\ell_{\sf min}$	0.67	0.57	0.64	0.06	0.58	0.55
$\ell_{\sf max}$	1.77	1.66	1.69	1.62	2.50	1.72
ℓ_{avg}	1.06	1.03	1.06	0.95	1.03	1.02
$\%\ell_{unit}$	99.10 %	99.92 %	99.06 %	89.60 %	96.48 %	99.74 %
q _{min}	0.47	0.09	0.46	0.10	0.09	0.17
q avg	0.90	0.90	0.90	0.80	0.83	0.90
%q _{unit}	92.15 %	93.46 %	92.08 %	62.45 %	67.44 %	92.25 %
# simplices	38.30k	42.67k	38.20k	58.62k	47.65k	43.60k

Visualizing slices of a 4*d* mesh







Why so much overshoot?



Valency statistics



Packing fraction

Packing fraction (ϕ) defined as volume fraction of space covered by particles.

Best known packing fractions of unit-length equilateral simplices [Kallus, 2011]:

 $\phi_{3} = 100/117 \approx 85.47\%$

 $\phi_4 = \texttt{128/219} \approx \texttt{58.45\%}$

Maintaining a valid mesh



Theory

Definition of a mesh topology:

Let \mathcal{V} be a set of vertices in some domain Ω and \mathcal{T} be a set of *n*-polytopes with vertices in \mathcal{V} . Let \mathcal{F} be the set of faces (n-1)-facets of \mathcal{T} . \mathcal{T} is called a *mesh topology* if

- (1) $\operatorname{card}(f \cap \mathcal{T}) \leq 2, \forall f \in \mathcal{F},$
- (2) $(\mathcal{V}, \partial \mathcal{T})$ is a mesh of $\partial \Omega$.

Practice

- (1) Close the mesh by connecting boundary to a ghost vertex.
- (2) Check inserted elements do not already exist in \mathcal{T} .
- (3) Use neighbour relations to ensure every facet touches two elements.



Convergence of the L^2 error for simple problem.



Adapting to L^2 error in solution:

 $u(x, y, z, t) = \exp(-5t)\sin 2\pi x \sin 2\pi y \sin 2\pi z$



Geometry metadata is important to determine validity of operators.



- Collapse edge e = (p, q): $g_q \preceq g_p$,
- Insert vertex p along edge $e: g_p \leftarrow g_e$,
- Swap edge e with re-insertion vertex p: $g_p \preceq g_e$,
- Smooth vertex *p*: driven by lengths of edges (p, q) surrounding *p* such that $g_q \leq g_p$.



Difference in 4*d* benchmarks with or without DOF control.



Property	Linear 1	Linear 2	Wave	Linear 1	Linear 2	Wave
	(no control)	(no control)	(no control)	(control)	(control)	(control)
$\ell_{\sf min}$	0.50	0.40	0.20	0.53	0.47	0.23
$\ell_{\sf max}$	1.91	1.86	2.71	1.78	1.96	2.99
ℓ_{avg}	1.08	1.08	1.08	1.10	1.11	1.12
%ℓ _{unit}	97.29 %	98.01 %	92.48 %	96.46 %	97.27 %	88.96 %
q _{min}	0.16	0.02	0.02	0.23	0.11	0.08
$q_{\rm avg}$	0.80	0.83	0.72	0.80	0.83	0.72
%q _{unit}	56.67 %	67.13 %	28.75 %	56.35 %	70.00 %	26.89 %
# simplices	59.56k	915.30k	394.07k	55.66k	814.50k	347.19k
expected	51.00k	818.00k	n/a	51.00k	818.00k	n/a

Mesh size and aspect ratio distributions for L^2 boundary layer case



Coefficient	Analytic	64k	128k	256k	512k
$h_{x,0}$	$h_{x,0}^{*}$	0.0155	0.0121	0.0095	0.0076
$h_{x,0}^{*}$	-	0.0090	0.0075	0.0063	0.0053
k _{hx}	43.75	25.14	28.39	31.29	33.74
$a_{y,0}$	50.00	25.52	29.46	32.15	33.76
k _{ay}	-50.00	-26.57	-31.14	-35.22	-38.05
$a_{z,0}$	25.00	14.32	16.02	17.09	18.18
kaz	-50.00	-26.84	-31.79	-35.92	-38.92
$a_{t,0}$	16.67	9.59	10.75	11.76	12.47
k_{a_t}	-50.00	-26.11	-31.44	-35.58	-39.25

Coefficient Analytic 64k 128k 256k 512k 0.0146 0.0119 0.0100 0.0081 $h_{x,0}$ $h_{x.0}^{*}$ 0.0125 0.0105 0.0088 0.0074 $h_{x,0}^{*}$ 30.00 25.46 24.56 27.36 28.00 k_{h_x} 38.06 42.92 40.45 44.13 50.00 $a_{y,0}$ -33.33 -24.69 -28.12 -29.80 -31.04 k_a, 25.00 22.41 21.51 22.11 22.06 $a_{z,0}$ -33.33 -25.96 -27.69 -30.55 -30.68 ka, 16.67 15.39 14.55 14.64 15.22 $a_{t,0}$ -33.33 -26.60 -28.50 -30.14 -31.74 ka,

p = 2

Advection-diffusion boundary layer convergence rates





Boundary layer (advection-diffusion) p = 2 meshes.





Spherical wave (advection-diffusion) p = 2 meshes.



