

Balancing Shape and Size: Asymptotic Analysis of Compound Volume+Shape Mesh Optimization Metrics

Tetrahedron VII: Seventh Workshop on Grid Generation for Numerical Computations, Barcelona, Spain.



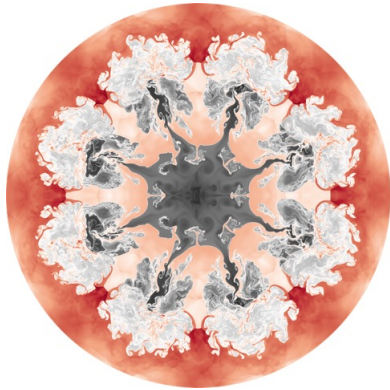
October 9-11, 2023

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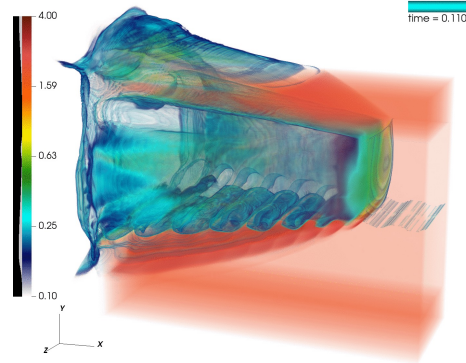


Framework – ALE for shock hydrodynamics through a high-order finite element code

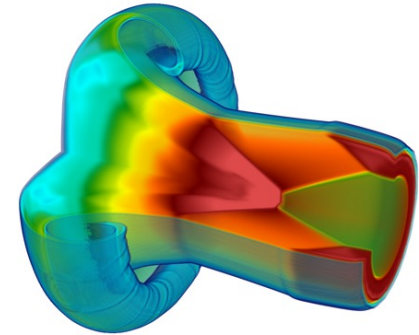
- We start with an established ALE shock hydro method (BLAST code at LLNL).



ICF perturbation test

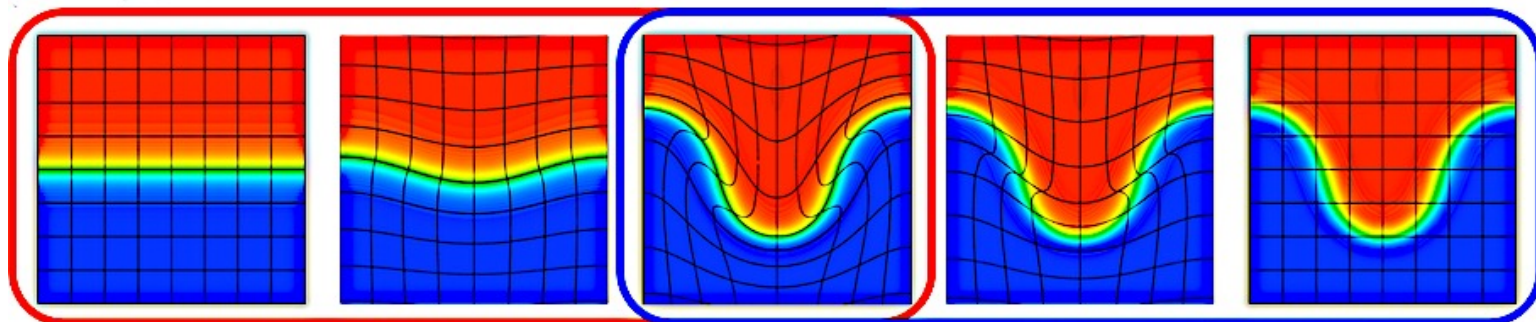


3D Radiation hydrodynamics



3D shock triple point interaction

- Mesh optimization as part of the ALE framework:

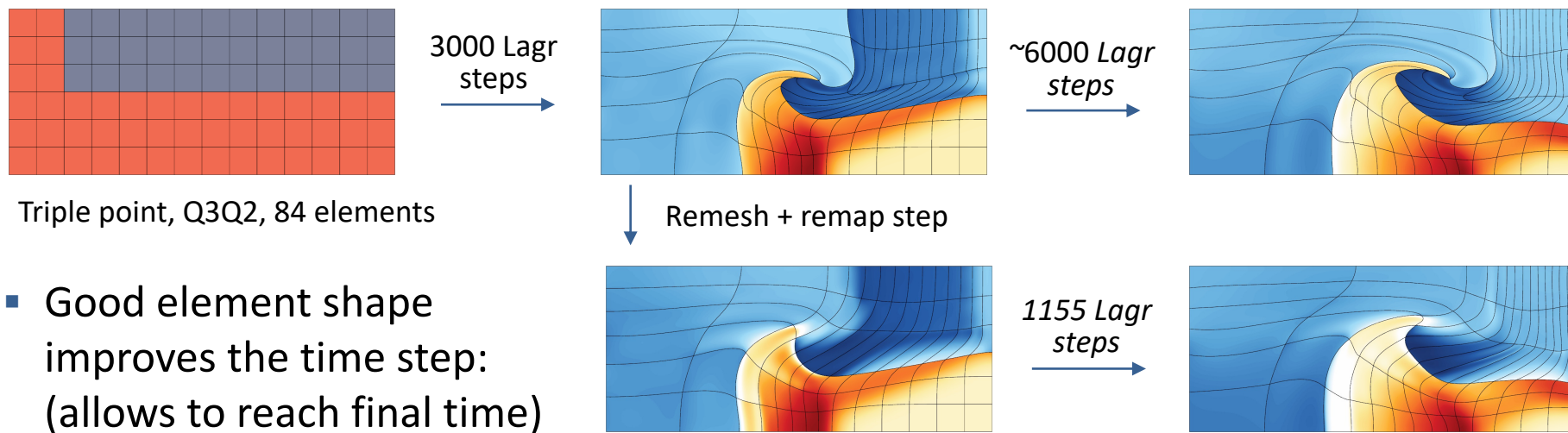


Lagrangian Phase

Remesh/Remap Phase

Main use case: r-adaptive mesh optimization in moving mesh simulations

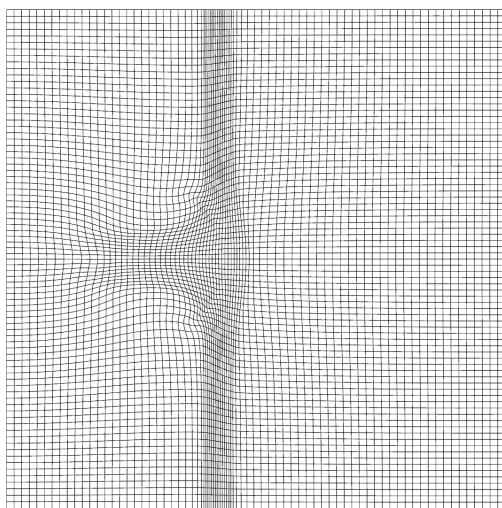
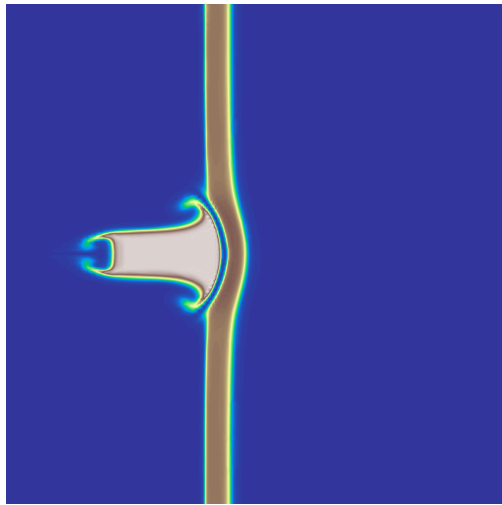
- Main application focus: ALE methods for shock hydrodynamics.



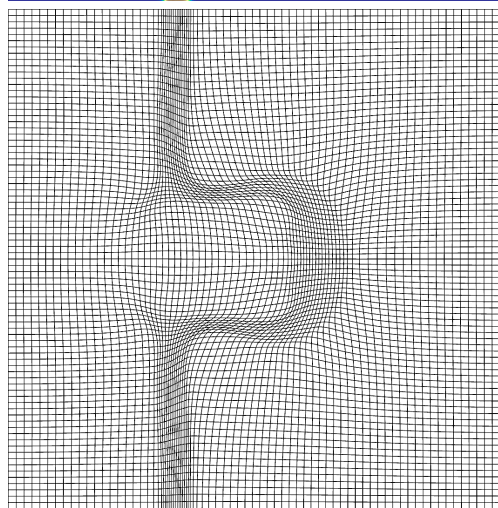
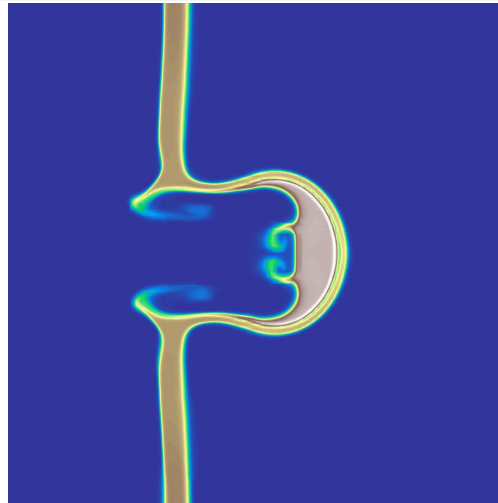
- Good element shape improves the time step: (allows to reach final time)
- Adapted size improves the accuracy.
- The optimizer must combine shape and size!

Method	Refs	Lagr Cycles	Runtime	# ALE	Error
Lagrangian	2	93 833	-	0	0
Lagrangian	1	18 482	266	0	0.069
Adapted to interfaces	1	1 577	54.4	19	0.099
Eulerian	2	1 508	134	21	0.098

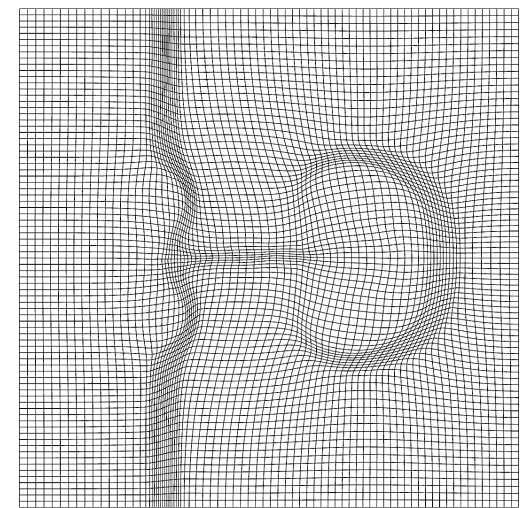
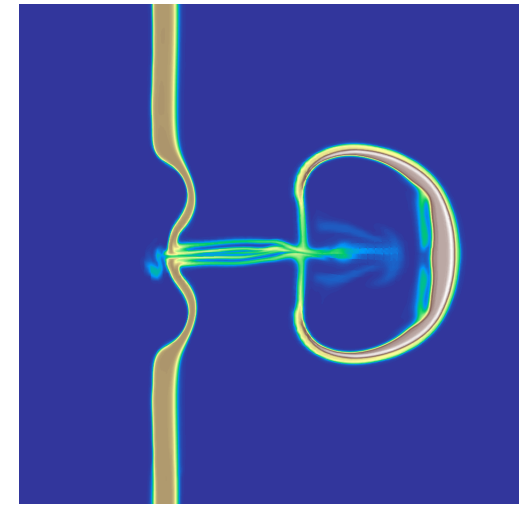
Main use case: r-adaptive mesh optimization in moving mesh simulations



$t = 2.0$



$t = 6.0$



$t = 10.0$

Approach overview: Target-Matrix Optimization Paradigm (TMOP) and variational minimization

- Target construction: the user defines ideal target elements by specifying the target Jacobians W .

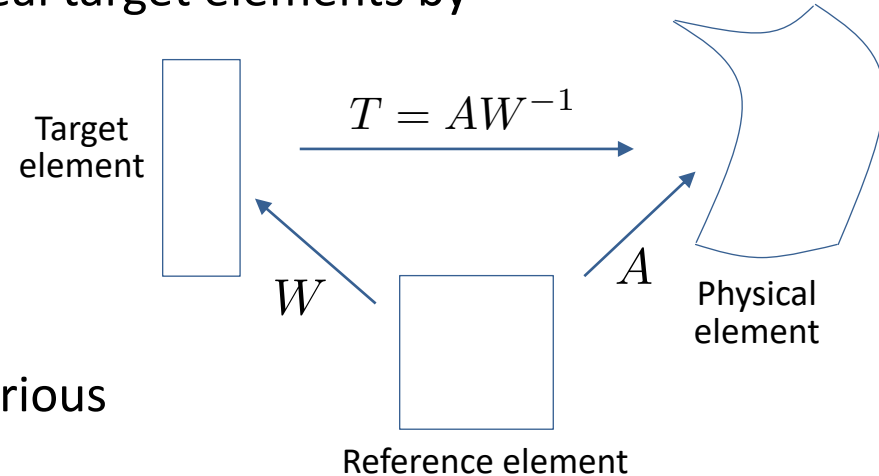
- The Jacobian T is used to define the local mesh quality measure $\mu(T)$.

- Combinations of W and $\mu(T)$ control various properties of the physical elements.

$W = [\text{volume}] [\text{orientation}] [\text{skew}] [\text{aspect ratio}]$.

- Variational minimization over the target elements (solving $\partial F(x) / \partial x = 0$):

$$F(x) := \sum_{E \in \mathcal{M}} \int_{E_t} \mu(T(x_t)) dx_t = \sum_{E \in \mathcal{M}} \sum_{x_q \in E_t} w_q \det(W(\bar{x}_q)) \mu(T(x_q))$$



Dobrev, Knupp, Kolev, Mittal, Tomov, “The Target-Matrix Optimization Paradigm for high-order meshes”, SISC, 2019

Knupp, “Metric Type in the Target-matrix Mesh Optimization Paradigm” LLNL-TR-817490, 2020.

TMOP mesh quality metrics

We have explored more than 60 metrics divided into 7 metric types

- Jacobian decomposition: $W = [\text{volume}] [\text{orientation}] [\text{skew}] [\text{aspect ratio}]$.

- Shape metrics – control over skew and aspect ratio.

Minimized when A is a scaled rotation of W .

$$\mu_2(T) = 0.5 \frac{|T|^2}{\det(T)} - 1$$

- Volume metrics – control over volume.

Minimized when $\det(A) = \det(W)$.

$$\mu_{77}(T) = 0.5 \left(\det(T) - \frac{1}{\det(T)} \right)^2$$

- Alignment metrics – control over orientation and skew.

Minimized when $A = W * \text{Diag}$.

$$\mu_{30}(A, W) = |\mathbf{a}_1| |\mathbf{w}_1| - (\mathbf{a}_1 \cdot \mathbf{w}_1) + |\mathbf{a}_2| |\mathbf{w}_2| - (\mathbf{a}_2 \cdot \mathbf{w}_2)$$

- Implicit combinations.

SH+V, SH+AL, V+AL, SH+V+AL.

$$\mu_7(T) = |T - T^{-t}|^2 \quad \mu_{14}(T) = |T - I|^2$$

- Explicit combinations.

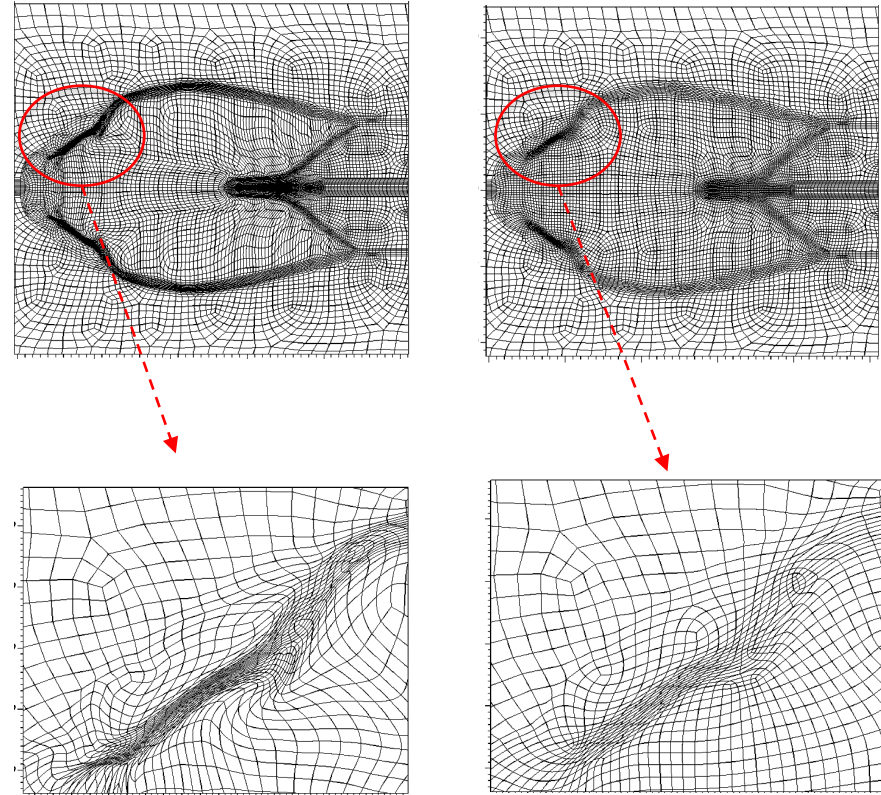
$$\mu(T) = \mu_i(T) + \gamma \mu_j(T)$$

P. Knupp, “Algebraic mesh quality metrics”, SIAM J. Sci. Comp., 23(1):193-218, 2001.

Problem statement: how to balance compound (explicit) volume+shape metrics

$$\mu(T) = \mu_s(T) + \lambda\mu_v(T)$$

- What is a good value for the weight?
- Originally, the weight decision was left to the user.
- Time consuming trial-error activity. Some tests require extreme values.
- Problem dependence (test case, adaptivity size ratio, refinement level). There's also time dependence in ALE.



Meshes optimized with different λ values.

Initial approach: compute weights through the properties of the initial mesh

$$\mu(T) = \frac{\bar{\mu}_v}{\bar{\mu}_s + \bar{\mu}_v} \mu_s(T) + \frac{\bar{\mu}_s}{\bar{\mu}_s + \bar{\mu}_v} \lambda \mu_v(T), \quad \bar{\mu}_v = \frac{1}{|\Omega_0|} \int_{\Omega_0} \mu_v(T)$$

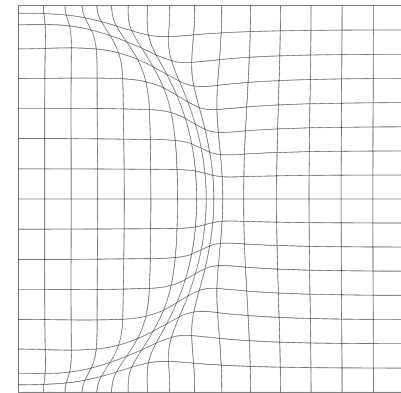
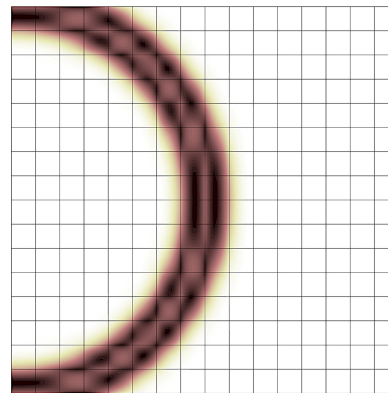
- Balances the magnitudes of the metrics based on the initial mesh.

Pros:

- Automatically adjusts weights based on the problem (and its initial mesh).
- Fits well the ALE framework, as weights are computed before each remesh.

Cons:

- Does not allow deterioration w.r.t. the initial shape / volume targets.
- Does not allow big shape deformations and extreme adaptivity.



Adaptivity to a discrete function, with ideal initial mesh

Additional requirements & considerations

- The balancing weight should not be problem-dependent.
- The method should allow big deformations w.r.t. the initial mesh. (deteriorate shape or size when needed)
- The weight should not be dynamic, as this affects the nonlinear solver.

Observations:

- The ratio between the magnitudes doesn't have a clear geometric meaning: $\mu_s = 10$ can be a slight shape deformation; $\mu_v = 2$ can be 2x volume error.
- The nonlinear objective is posed w.r.t. the gradients of the metrics.

$$\frac{\partial}{\partial x} \int_{\Omega} \mu_s(x) + \lambda \mu_v(x) = 0$$

- All this suggests to look at the asymptotic behavior of the metrics.

2D asymptotic limits are computed through the extreme values of the geometric parameters

- Geometric parameters (no rotation): two lengths (a , b) and a skew angle (ϕ).

$$A = \begin{pmatrix} a & b \cos \phi \\ 0 & b \sin \phi \end{pmatrix}$$

$$v = \det(A) = a b \sin \phi$$

$$|A|^2 = a^2 + b^2$$

Case	Description	Consequences
1a	$a \rightarrow \infty; b = 1; \sin \phi = 1$	$v = a \rightarrow \infty$
1b	$b \rightarrow \infty; a = 1; \sin \phi = 1$	$v = b \rightarrow \infty$
2a	$a \rightarrow 0; b = 1; \sin \phi = 1$	$v = a \rightarrow 0$
2b	$b \rightarrow 0; a = 1; \sin \phi = 1$	$v = b \rightarrow 0$
3	$\sin \phi \rightarrow 0; a = b = 1$	$v = \sin \phi \rightarrow 0$

Asymptotic cases for 2D Jacobians

- Procedure: for a given metric, for each case compute the limits in w.r.t. v .

$$\begin{aligned} \mu_2 &= \frac{|A|^2}{2 \det(A)} - 1, & \mu_2 &= \frac{a^2 + b^2}{2 a b \sin \phi} - 1, \\ \mu_{50} &= \frac{|A^t A|^2}{2 [\det(A)]^2} - 1. & \mu_{50} &= \frac{a^4 + 2 a^2 b^2 \cos^2 \phi + b^4}{2 a^2 b^2 \sin^2 \phi} - 1. \end{aligned}$$

Case	μ_2	μ_{50}
1a, 1b	$\frac{v}{2}$	$\frac{v^2}{2}$
2a, 2b	$\frac{1}{2v}$	$\frac{1}{2v^2}$
3	$\frac{1}{v}$	$\frac{2}{v^2}$

Asymptotics of 2D shape metrics

- Same is done for volume metrics, and the limits are compared.

Matching of the asymptotic limits reveals which compound volume+shape metrics are balanced

- Considered volume metrics: $\mu_{56} = \frac{1}{2} \left(v + \frac{1}{v} \right) - 1$,
 $\mu_{77} = \frac{1}{2} \left(v^2 + \frac{1}{v^2} \right) - 1$.

Case	μ_{56}	μ_{77}
1a, 1b	$\frac{v}{2}$	$\frac{v^2}{2}$
2a, 2b	$\frac{1}{2v}$	$\frac{1}{2v^2}$
3	$\frac{1}{2v}$	$\frac{1}{2v^2}$

Asymptotics of 2D volume metrics

- Match μ_2 +size:

Case	μ_2	μ_{56}	Relation
1	$\frac{v}{2}$	$\frac{v}{2}$	$\mu_{56} = \mu_2$
2	$\frac{1}{2v}$	$\frac{1}{2v}$	$\mu_{56} = \mu_2$
3	$\frac{1}{v}$	$\frac{1}{2v}$	$\mu_{56} = \frac{\mu_2}{2}$

$$\mu_{94} = \mu_2 + \lambda \mu_{56}, \text{ with } 1 \leq \lambda \leq 2.$$

- Match μ_{50} +size:

Case	μ_{50}	μ_{56}	Relation
1	$\frac{v^2}{2}$	$\frac{v}{2}$	$\mu_{50} = 2 \mu_{56}^2$
2	$\frac{1}{2v^2}$	$\frac{1}{2v}$	$\mu_{50} = 2 \mu_{56}^2$
3	$\frac{2}{v^2}$	$\frac{1}{2v}$	$\mu_{50} = 8 \mu_{56}^2$

$$\overline{\mu_{53}} = \mu_{50} + \lambda \mu_{56}^2, \text{ with } 2 \leq \lambda \leq 8.$$

Case	μ_2	μ_{77}	Relation
1	$\frac{v}{2}$	$\frac{v^2}{2}$	$\mu_{77} = 2 \mu_2^2$
2	$\frac{1}{2v}$	$\frac{1}{2v^2}$	$\mu_{77} = 2 \mu_2^2$
3	$\frac{1}{v}$	$\frac{1}{2v^2}$	$\mu_{77} = \frac{1}{2} \mu_2^2$

$$\overline{\mu_{80}} = \mu_2^2 + \lambda \mu_{77}, \text{ with } \frac{1}{2} \leq \lambda \leq 2.$$

Case	μ_{50}	μ_{77}	Relation
1	$\frac{v^2}{2}$	$\frac{v^2}{2}$	$\mu_{50} = \mu_{77}$
2	$\frac{1}{2v^2}$	$\frac{1}{2v^2}$	$\mu_{50} = \mu_{77}$
3	$\frac{2}{v^2}$	$\frac{1}{2v^2}$	$\mu_{50} = 4 \mu_{77}$

$$\mu_{90} = \mu_{50} + \lambda \mu_{77}, \text{ with } 1 \leq \lambda \leq 4.$$

- The procedure can be applied to any type of compound metric.

3D geometric parameters & asymptotic limits

- Geometric parameters (no rotation): two lengths and three angles.

$$A = \begin{pmatrix} 1 & a \cos \phi & b \cos \psi \\ 0 & a \sin \phi & b \sin \psi \cos \chi \\ 0 & 0 & b \sin \psi \sin \chi \end{pmatrix}$$

$$v = \zeta \sin \phi \sin \psi \sin \chi$$

$$|A|^2 = 1 + a^2 + b^2$$

$$|adj A|^2 = a^2 \sin^2 \phi + b^2 \sin^2 \psi + a^2 b^2 (\cos \phi \sin \psi \cos \chi - \sin \phi \cos \psi)^2 + a^2 b^2 \sin^2 \psi \sin^2 \chi.$$

Case	a	b	$\sin \phi$	$\sin \psi$	$\sin \chi$	$ A ^2$	$ adj A ^2$	$\kappa^2(A)$	v
1	1	1	1	1	$\rightarrow 0$	3	2	$\frac{6}{v^2}$	$\rightarrow 0$
2	1	1	1	$\rightarrow 0$	1	3	2	$\frac{6}{v^2}$	$\rightarrow 0$
3	1	1	$\rightarrow 0$	1	1	3	2	$\frac{6}{v^2}$	$\rightarrow 0$
4	$\rightarrow \infty$	1	1	1	1	$\rightarrow a^2$	$2a^2$	$2v^2$	$\rightarrow a$
5	$\rightarrow 0$	1	1	1	1	2	1	$\frac{2}{v^2}$	$\rightarrow 0$
6	1	$\rightarrow \infty$	1	1	1	$\rightarrow b^2$	$2b^2$	$2v^2$	$\rightarrow b$
7	1	$\rightarrow 0$	1	1	1	2	1	$\frac{2}{v^2}$	$\rightarrow 0$

Asymptotic cases for 3D Jacobians

3D shape / volume metrics and their asymptotics

- Considered shape metrics:

$$\mu_{301} = \frac{1}{3} \kappa(A) - 1 = \frac{1}{3} |A| |adj A| - 1,$$

$$\mu_{302} = \frac{1}{9} \kappa^2(A) - 1 = \frac{1}{9} |A|^2 |adj A|^2 - 1,$$

$$\mu_{303} = \frac{|A|^2}{3v^{2/3}} - 1,$$

$$\mu_{304} = \frac{|A|^3}{3\sqrt{3}v} - 1.$$

Case	μ_{301}	μ_{302}	μ_{303}	μ_{304}
1	$\frac{\sqrt{6}}{3v}$	$\frac{2}{3v^2}$	$\frac{1}{v^{2/3}}$	$\frac{1}{v}$
2	$\frac{\sqrt{6}}{3v}$	$\frac{2}{3v^2}$	$\frac{1}{v^{2/3}}$	$\frac{1}{v}$
3	$\frac{\sqrt{6}}{3v}$	$\frac{2}{3v^2}$	$\frac{1}{v^{2/3}}$	$\frac{1}{v}$
4	$\frac{\sqrt{2}v}{3}$	$\frac{2v^2}{9}$	$\frac{v^{4/3}}{3}$	$\frac{v^2}{3\sqrt{3}}$
5	$\frac{\sqrt{2}}{3v}$	$\frac{2}{9v^2}$	$\frac{2}{3v^{2/3}}$	$\left(\frac{2}{3}\right)^{\frac{3}{2}} \cdot \frac{1}{v}$
6	$\frac{\sqrt{2}v}{3}$	$\frac{2v^2}{9}$	$\frac{v^{4/3}}{3}$	$\frac{v^2}{3\sqrt{3}}$
7	$\frac{\sqrt{2}}{3v}$	$\frac{2}{9v^2}$	$\frac{2}{3v^{2/3}}$	$\left(\frac{2}{3}\right)^{\frac{3}{2}} \cdot \frac{1}{v}$

Asymptotics of 3D shape metrics

- Considered volume metrics:

$$\mu_{316} = \frac{1}{2} \left(\sqrt{v} - \frac{1}{\sqrt{v}} \right)^2 = \frac{1}{2} \left(v + \frac{1}{v} \right) - 1,$$

$$\mu_{318} = \frac{1}{2} \left(v - \frac{1}{v} \right)^2 = \frac{1}{2} \left(v^2 + \frac{1}{v^2} \right) - 1.$$

Case	v	μ_{316}	μ_{318}
1	$\rightarrow 0$	$\frac{1}{2v}$	$\frac{1}{2v^2}$
2	$\rightarrow 0$	$\frac{1}{2v}$	$\frac{1}{2v^2}$
3	$\rightarrow 0$	$\frac{1}{2v}$	$\frac{1}{2v^2}$
4	$\rightarrow a$	$\frac{v}{2}$	$\frac{v^2}{2}$
5	$\rightarrow 0$	$\frac{1}{2v}$	$\frac{1}{2v^2}$
6	$\rightarrow b$	$\frac{v}{2}$	$\frac{v^2}{2}$
7	$\rightarrow 0$	$\frac{1}{2v}$	$\frac{1}{2v^2}$

Asymptotics of 3D volume metrics

3D volume+shape compound metrics

- Match μ_{301} +size:

Cases	μ_{301}	μ_{316}	Compound	μ_{318}	Compound
1, 2, 3	$\frac{\sqrt{6}}{3v}$	$\frac{1}{2v}$	$\frac{3}{8}\mu_{301} + \mu_{316}$	$\frac{1}{2v^2}$	$\mu_{301}^2 + \frac{4}{3}\mu_{318}$
4, 6	$\frac{\sqrt{2}v}{3}$	$\frac{v}{2}$	$\frac{9}{8}\mu_{301} + \mu_{316}$	$\frac{v^2}{2}$	$\mu_{301}^2 + \frac{4}{9}\mu_{318}$
5, 7	$\frac{\sqrt{2}}{3v}$	$\frac{1}{2v}$	$\frac{9}{8}\mu_{301} + \mu_{316}$	$\frac{1}{2v^2}$	$\mu_{301}^2 + \frac{4}{9}\mu_{318}$
All			$\lambda\mu_{301} + \mu_{316}$		$\mu_{301}^2 + \lambda\mu_{318}$

Suggested Compound Metric is $\mu_{370} = \mu_{301} + \lambda\mu_{316}$, with $\frac{3}{8} \leq \lambda \leq \frac{9}{8}$

- Match μ_{302} +size:

Cases	μ_{302}	μ_{316}	Compound	μ_{318}	Compound
1, 2, 3	$\frac{2}{3v^2}$	$\frac{1}{2v}$	$\frac{3}{8}\mu_{302} + \mu_{316}^2$	$\frac{1}{2v^2}$	$\mu_{302} + 3\mu_{318}$
4, 6	$\frac{2v^2}{9}$	$\frac{v}{2}$	$\frac{9}{8}\mu_{302} + \mu_{316}^2$	$\frac{v^2}{2}$	$\mu_{302} + \frac{4}{9}\mu_{318}$
5, 7	$\frac{2}{9v^2}$	$\frac{1}{2v}$	$\frac{9}{8}\mu_{302} + \mu_{316}^2$	$\frac{1}{2v^2}$	$\mu_{302} + \frac{4}{9}\mu_{318}$
All			$\lambda\mu_{302} + \mu_{316}^2$		$\mu_{302} + \lambda\mu_{318}$

Suggested Compound Metric is $\mu_{338} = \mu_{302} + \lambda\mu_{318}$, with $\frac{4}{9} \leq \lambda \leq 3$

3D volume+shape compound metrics

- Match μ_{303} +size:

Cases	μ_{303}	μ_{316}	Compound	μ_{318}	Compound
1, 2, 3	$\frac{1}{v^{2/3}}$	$\frac{1}{2v}$	$\mu_{303} + (2\mu_{316})^{2/3}$	$\frac{1}{2v^2}$	$\mu_{303}^3 + 2\mu_{318}$
4, 6	$\frac{v^{4/3}}{3}$	$\frac{v}{2}$	$3\mu_{303} + (2\mu_{316})^{4/3}$	$\frac{v^2}{2}$	$(3\mu_{303})^{3/2} + 2\mu_{318}$
5, 7	$\frac{2}{3v^{2/3}}$	$\frac{1}{2v}$	$\frac{3}{2}\mu_{303} + (2\mu_{316})^{2/3}$	$\frac{1}{2v^2}$	$(\frac{3}{2}\mu_{303})^3 + 2\mu_{318}$
All			$\lambda\mu_{303} + (2\mu_{316})^p$		$(\lambda\mu_{303})^p + 2\mu_{318}$

It is not possible to match the shape and volume asymptotic limits

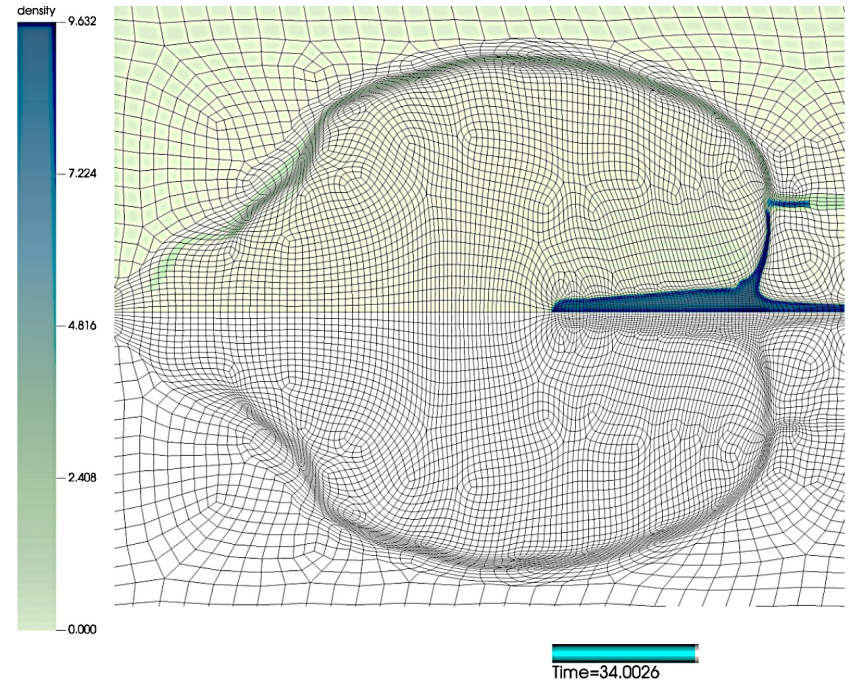
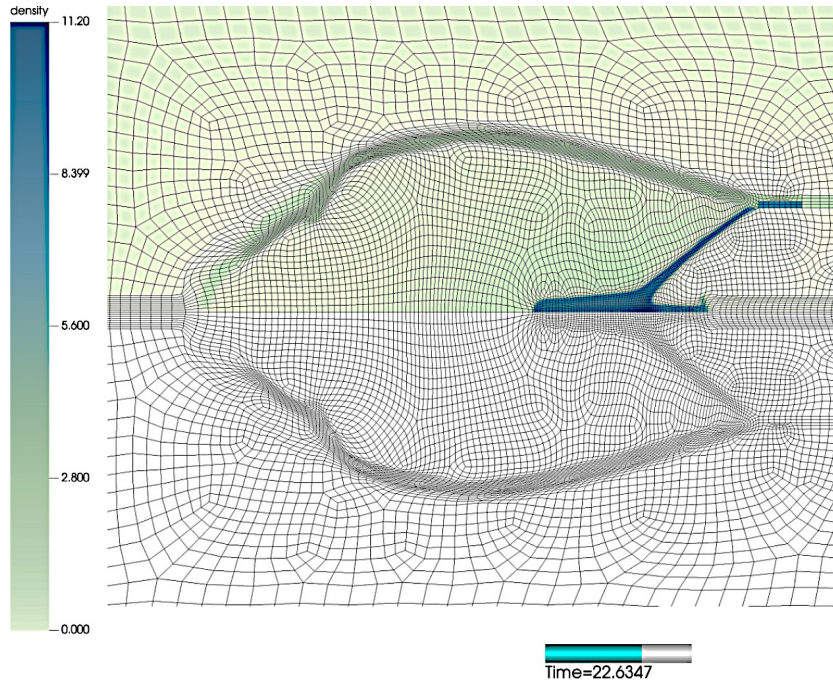
- Match μ_{304} +size:

Cases	μ_{304}	μ_{316}	Compound	μ_{318}	Compound
1, 2, 3	$\frac{1}{v}$	$\frac{1}{2v}$	$\mu_{304} + 2\mu_{316}$	$\frac{1}{2v^2}$	$\mu_{304}^2 + 2\mu_{318}$
4, 6	$\frac{v^2}{3\sqrt{3}}$	$\frac{v}{2}$	$\mu_{304} + \left(\frac{4}{3\sqrt{3}}\right)\mu_{316}^2$	$\frac{v^2}{2}$	$\mu_{304} + \left(\frac{2}{3\sqrt{3}}\right)\mu_{318}$
5, 7	$\left(\frac{2}{3}\right)^{\frac{3}{2}} \cdot \frac{1}{v}$	$\frac{1}{2v}$	$\mu_{304} + 2\left(\frac{2}{3}\right)^{\frac{3}{2}}\mu_{316}$	$\frac{1}{2v^2}$	$\mu_{304}^2 + 2\left(\frac{2}{3}\right)^3\mu_{318}$
All			$\mu_{304} + \lambda\mu_{316}^p$		$\mu_{304}^p + \lambda\mu_{318}$

It is not possible to match the shape and volume asymptotic limits

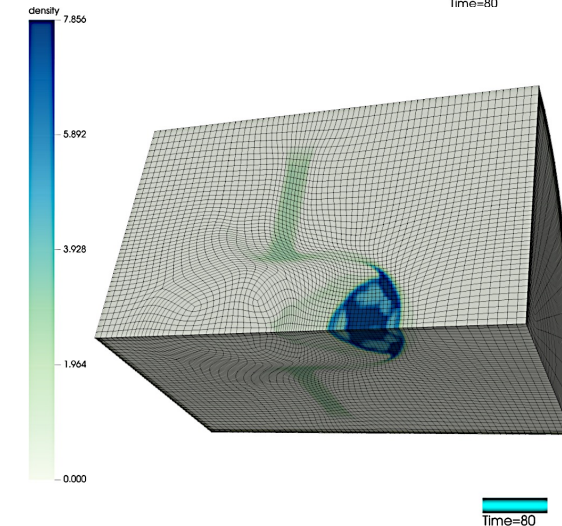
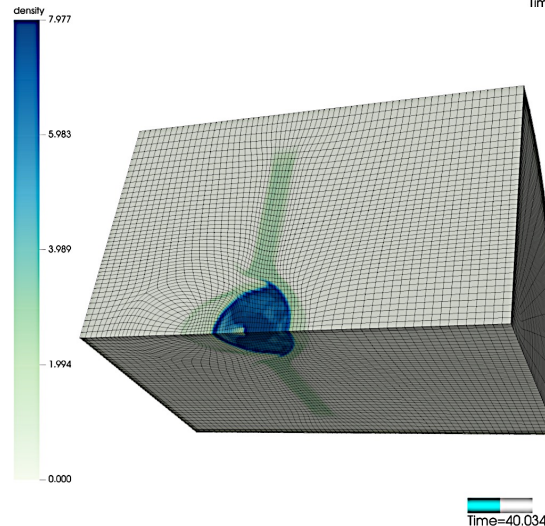
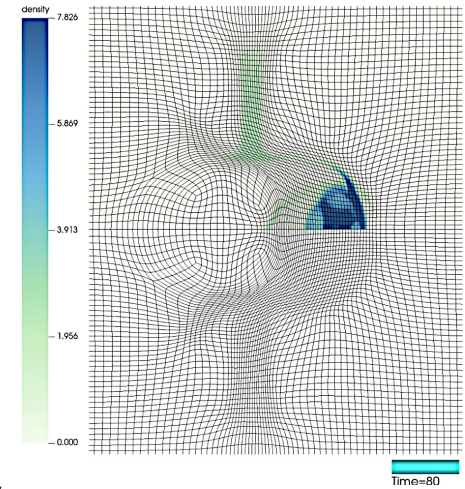
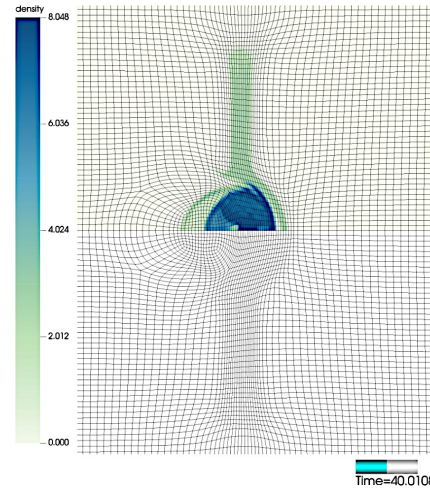
Application results – 2D shaped charge

- Computed by μ_{94} with $\lambda = 1.5$ (the default weight)
- Targets 3:1 volume ratio.
- Previously computed by a non-balanced metric, resulting in many trials / errors.



Application results – 2D & 3D ball impact

- Computed by μ_{94} with $\lambda = 1.5$ (the default weight)
- Targets 2:1 volume ratio.
- Computed by μ_{338} with $\lambda = 0.1 * \text{default}$.
- Puts more emphasis on element shape



Summary

- Asymptotic analysis to derive balanced composite volume+shape metrics.

$$\mu_{94} = \mu_2 + \lambda \mu_{56}$$

$$\mu_{338} = \mu_{302} + \lambda \mu_{318}$$

$$\mu_{90} = \mu_{50} + \lambda \mu_{77}$$

$$\mu_{370} = \mu_{301} + \lambda \mu_{316}$$

- The analysis provides problem-independent defaults.
- Some of the previously used metrics turned out to be unbalanced.
- Alleviates the trial & error weight adjustments in practical simulations.

Modular Finite Element Methods (MFEM)

Flexible discretizations on unstructured grids

- Triangular, quadrilateral, tetrahedral, hexahedral, prism; volume, surface and topologically periodic meshes
- Bilinear/linear forms for: Galerkin methods, DG, HDG, DPG, IGA, ...
- Local conforming and non-conforming AMR, mesh optimization

High-order methods and scalability

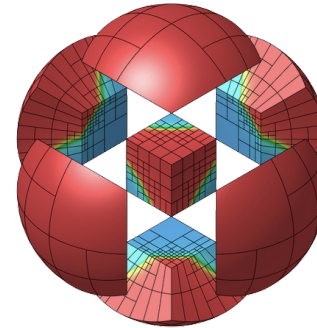
- Arbitrary-order H1, H(curl), H(div)- and L2 elements
- Arbitrary order curvilinear meshes
- MPI scalable to millions of cores + GPU accelerated
- Enables development from laptops to exascale machines.

Solvers and preconditioners

- Integrated with: HYPRE, SUNDIALS, PETSc, SLEPc, SUPERLU, VisIt, ...
- AMG solvers for full de Rham complex on CPU+GPU, geometric MG
- Time integrators: SUNDIALS, PETSc, built-in RK, SDIRK, ...

Open-source software

- Open-source (GitHub) with 114 contributors, 50 clones/day
- Part of FASTMath, ECP/CEED, xSDK, OpenHPC, E4S, ...
- 75+ example codes & miniapps: mfem.org/examples



mfem.org
(v4.6, Sep/2023)

2023 workshop



radius



CEED
EXASCALE DISCRETIZATIONS



NUMFOCUS
OPEN CODE = BETTER SCIENCE

openHPC





CASC

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Scientific Computing

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