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.

CASC
Center for Applied Scientific Computing

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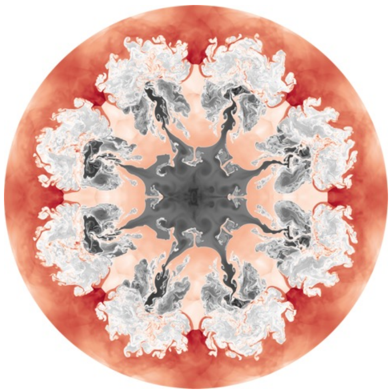
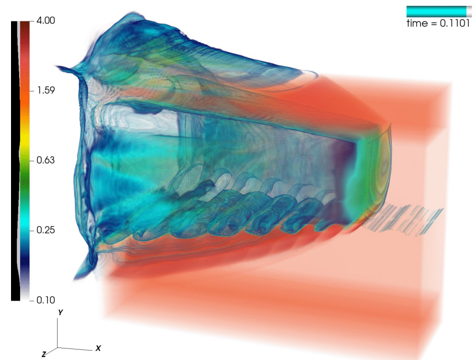
Framework – ALE for shock hydrodynamics through a high-order finite element code

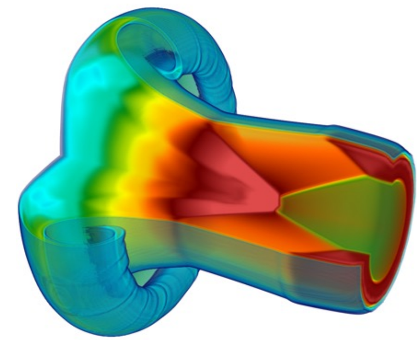
- We start with an established ALE shock hydro method (BLAST code at LLNL).



ICF perturbation test

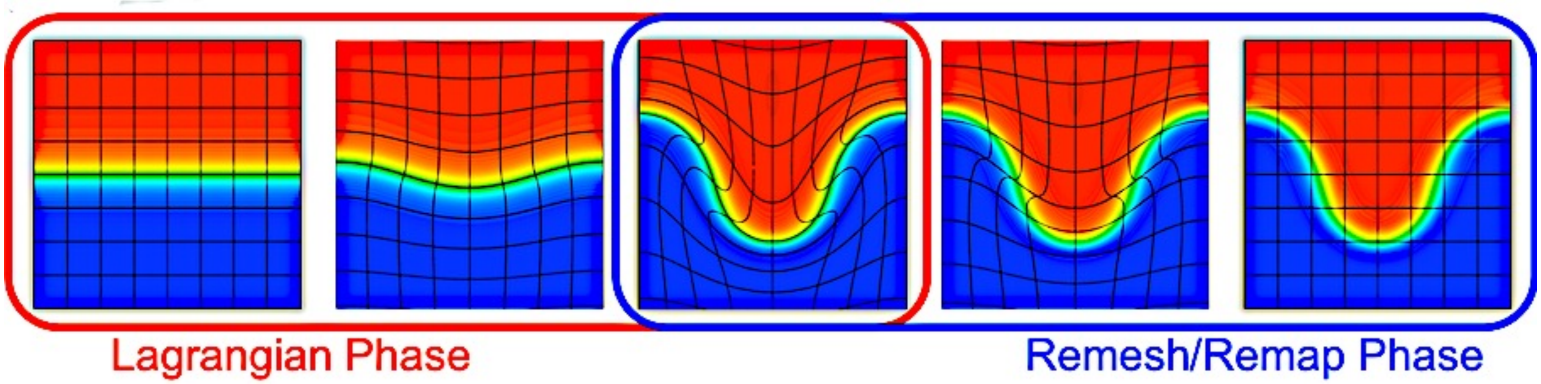


3D Radiation hydrodynamics



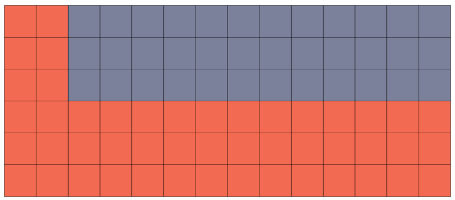
3D shock triple point interaction

- Mesh optimization as part of the ALE framework:



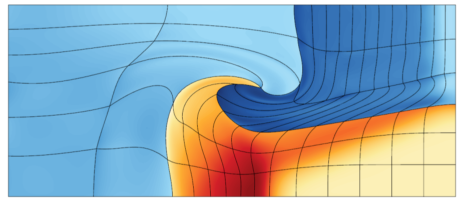
Main use case: r-adaptive mesh optimization in moving mesh simulations

- Main application focus: ALE methods for shock hydrodynamics.

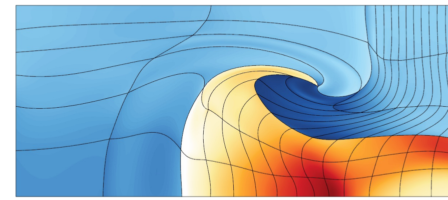


Triple point, Q3Q2, 84 elements

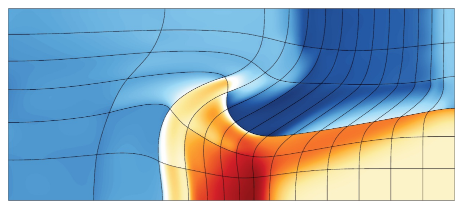
3000 Lagr steps →



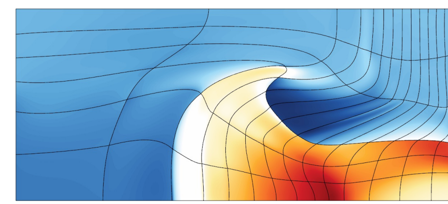
~6000 Lagr steps →



↓ Remesh + remap step



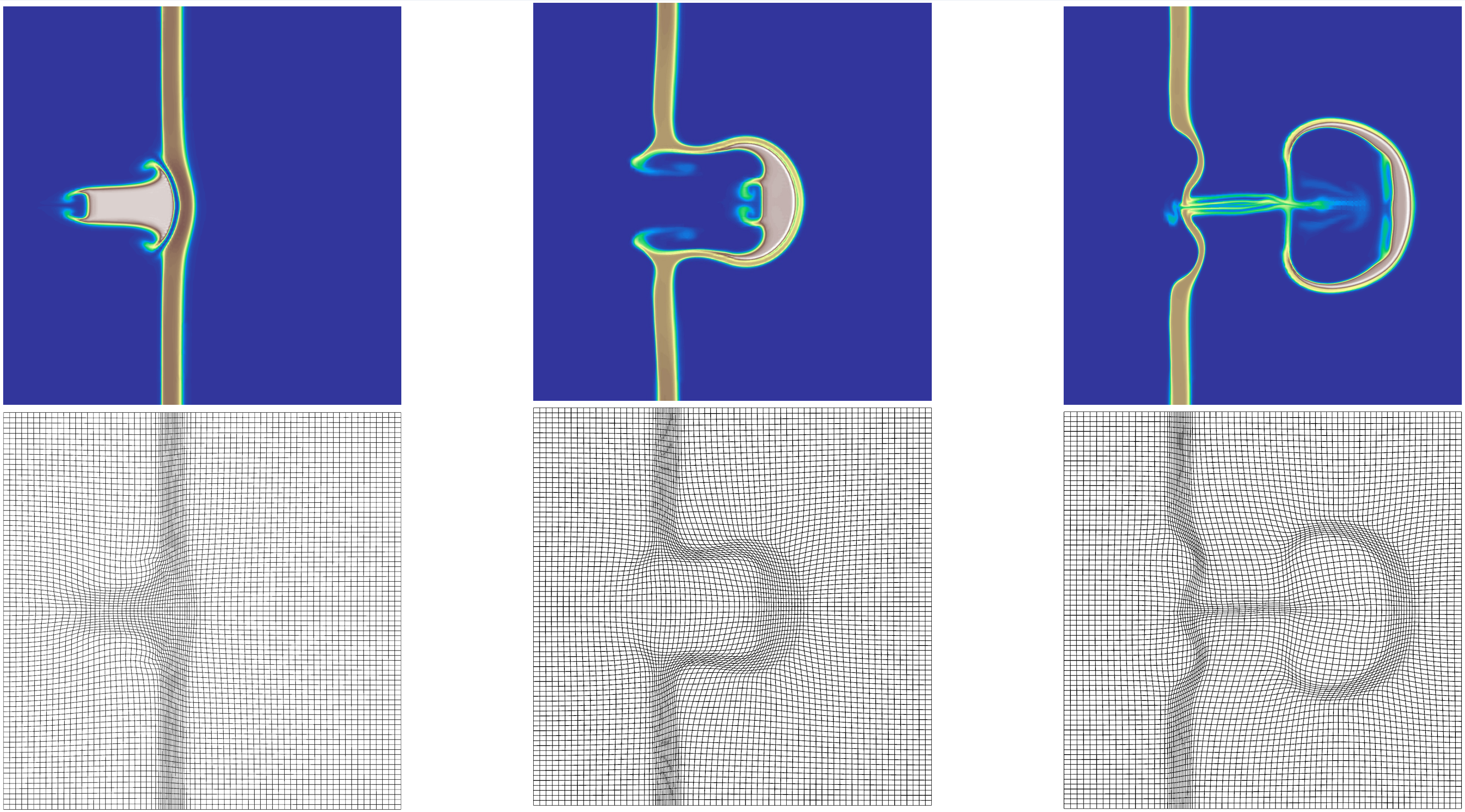
1155 Lagr steps →



- 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

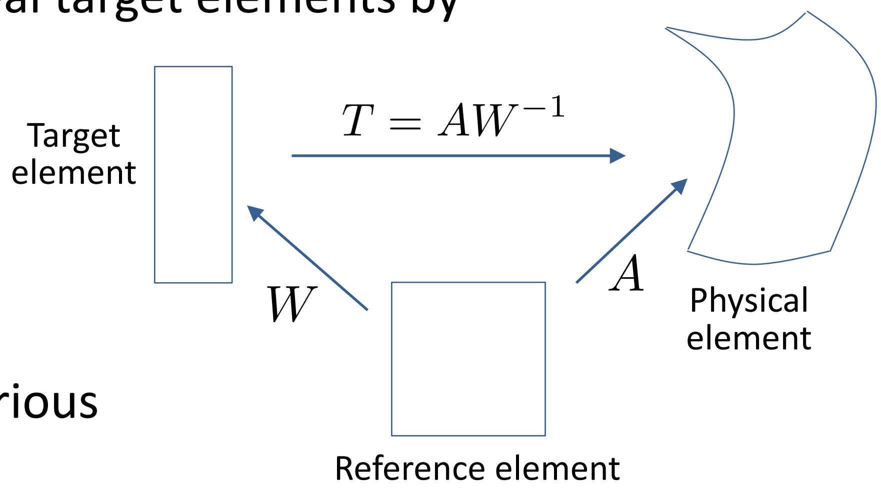
Main use case: r-adaptive mesh optimization in moving mesh simulations



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.
  $W =$ [volume] [orientation] [skew] [aspect ratio].
- Variational minimization over the target elements (solving $\partial F(x) / \partial \boldsymbol{x} = 0$):

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

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: $W =$ [volume] [orientation] [skew] [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 $A = \mathrm{W} * \mathrm{Diag}$.

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

- Implicit combinations.
  SH+V, SH+AL, V+AL, SH+V+AL.

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

- Explicit combinations.

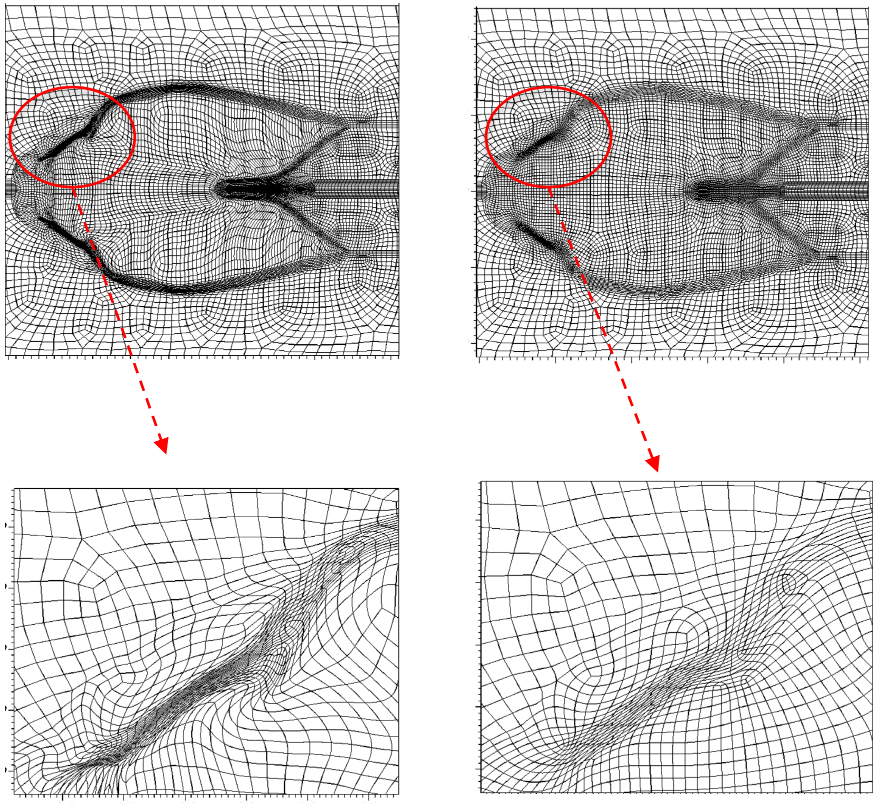
$$\mu(T) = \mu_i(T) + \gamma\mu_j(T)$$

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

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

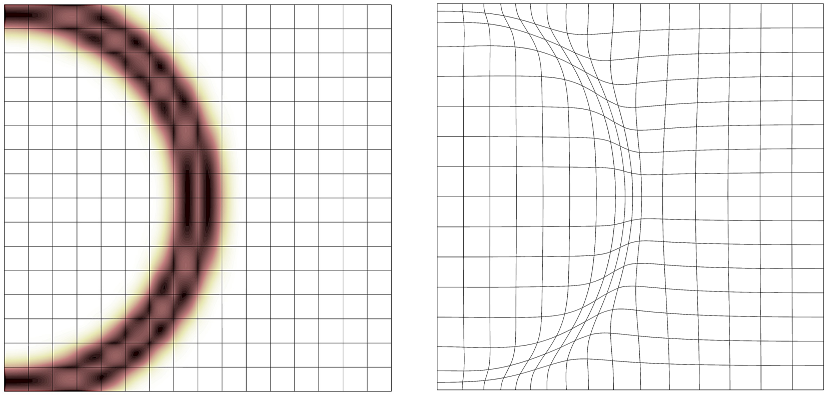
- Balances the magnitudes of the metrics based on the initial mesh.

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).

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

$$\upsilon = det(A) = a\,b\,\sin\phi$$

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

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

Asymptotic cases for 2D Jacobians

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

$$\mu_2 = \frac{|\,A\,|^2}{2\,det(A)} - 1, \qquad \mu_2 = \frac{a^2 + b^2}{2\,a\,b\,\sin\phi} - 1,$$

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

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

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

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

Asymptotics of 2D volume metrics

- Match μ_2+size:

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

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

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

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

- Match μ_{50}+size:

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

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

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

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

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

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

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

$$\begin{aligned} |adj\,A|^2 &= a^2\sin^2\phi + b^2\sin^2\psi \\ &+ a^2b^2(\cos\phi\sin\psi\cos\chi - \sin\phi\cos\psi)^2 \\ &+ a^2b^2\sin^2\psi\sin^2\chi. \end{aligned}$$

Case	a	b	$\sin\phi$	$\sin\psi$	$\sin\chi$	$\|A\|^2$	$\|adj\,A\|^2$	$\kappa^2(A)$	υ
1	1	1	1	1	$\to 0$	3	2	$\frac{6}{\upsilon^2}$	$\to 0$
2	1	1	1	$\to 0$	1	3	2	$\frac{6}{\upsilon^2}$	$\to 0$
3	1	1	$\to 0$	1	1	3	2	$\frac{6}{\upsilon^2}$	$\to 0$
4	$\to \infty$	1	1	1	1	$\to a^2$	$2a^2$	$2\upsilon^2$	$\to a$
5	$\to 0$	1	1	1	1	2	1	$\frac{2}{\upsilon^2}$	$\to 0$
6	1	$\to \infty$	1	1	1	$\to b^2$	$2b^2$	$2\upsilon^2$	$\to b$
7	1	$\to 0$	1	1	1	2	1	$\frac{2}{\upsilon^2}$	$\to 0$

Asymptotic cases for 3D Jacobians

3D shape / volume metrics and their asymptotics

- Considered shape metrics:

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

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

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

$$\mu_{304} = \frac{\mid A \mid^3}{3\sqrt{3}\,\upsilon} - 1.$$

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

Asymptotics of 3D shape metrics

- Considered volume metrics:

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

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

Case	υ	μ_{316}	μ_{318}
1	$\to 0$	$\frac{1}{2\,\upsilon}$	$\frac{1}{2\,\upsilon^2}$
2	$\to 0$	$\frac{1}{2\,\upsilon}$	$\frac{1}{2\,\upsilon^2}$
3	$\to 0$	$\frac{1}{2\,\upsilon}$	$\frac{1}{2\,\upsilon^2}$
4	$\to a$	$\frac{\upsilon}{2}$	$\frac{\upsilon^2}{2}$
5	$\to 0$	$\frac{1}{2\,\upsilon}$	$\frac{1}{2\,\upsilon^2}$
6	$\to b$	$\frac{\upsilon}{2}$	$\frac{\upsilon^2}{2}$
7	$\to 0$	$\frac{1}{2\,\upsilon}$	$\frac{1}{2\,\upsilon^2}$

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	$\frac{\sqrt{6}}{3\,\upsilon}$	$\frac{1}{2\,\upsilon}$	$\frac{3}{8}\,\mu_{301} + \mu_{316}$	$\frac{1}{2\,\upsilon^2}$	$\mu_{301}^2 + \frac{4}{3}\,\mu_{318}$
4, 6	$\frac{\sqrt{2}\,\upsilon}{3}$	$\frac{\upsilon}{2}$	$\frac{9}{8}\,\mu_{301} + \mu_{316}$	$\frac{\upsilon^2}{2}$	$\mu_{301}^2 + \frac{4}{9}\,\mu_{318}$
5, 7	$\frac{\sqrt{2}}{3\,\upsilon}$	$\frac{1}{2\,\upsilon}$	$\frac{9}{8}\,\mu_{301} + \mu_{316}$	$\frac{1}{2\,\upsilon^2}$	$\mu_{301}^2 + \frac{4}{9}\,\mu_{318}$
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	$\frac{2}{3\,\upsilon^2}$	$\frac{1}{2\,\upsilon}$	$\frac{3}{8}\,\mu_{302} + \mu_{316}^2$	$\frac{1}{2\,\upsilon^2}$	$\mu_{302} + 3\,\mu_{318}$
4, 6	$\frac{2\,\upsilon^2}{9}$	$\frac{\upsilon}{2}$	$\frac{9}{8}\,\mu_{302} + \mu_{316}^2$	$\frac{\upsilon^2}{2}$	$\mu_{302} + \frac{4}{9}\,\mu_{318}$
5, 7	$\frac{2}{9\,\upsilon^2}$	$\frac{1}{2\,\upsilon}$	$\frac{9}{8}\,\mu_{302} + \mu_{316}^2$	$\frac{1}{2\,\upsilon^2}$	$\mu_{302} + \frac{4}{9}\,\mu_{318}$
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	$\frac{1}{v^{2/3}}$	$\frac{1}{2\,v}$	$\mu_{303} + (2\,\mu_{316})^{2/3}$	$\frac{1}{2\,v^2}$	$\mu_{303}^3 + 2\,\mu_{318}$
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	$\frac{2}{3\,v^{2/3}}$	$\frac{1}{2\,v}$	$\frac{3}{2}\,\mu_{303} + (2\,\mu_{316})^{2/3}$	$\frac{1}{2\,v^2}$	$\left(\frac{3}{2}\,\mu_{303}\right)^3 + 2\,\mu_{318}$
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

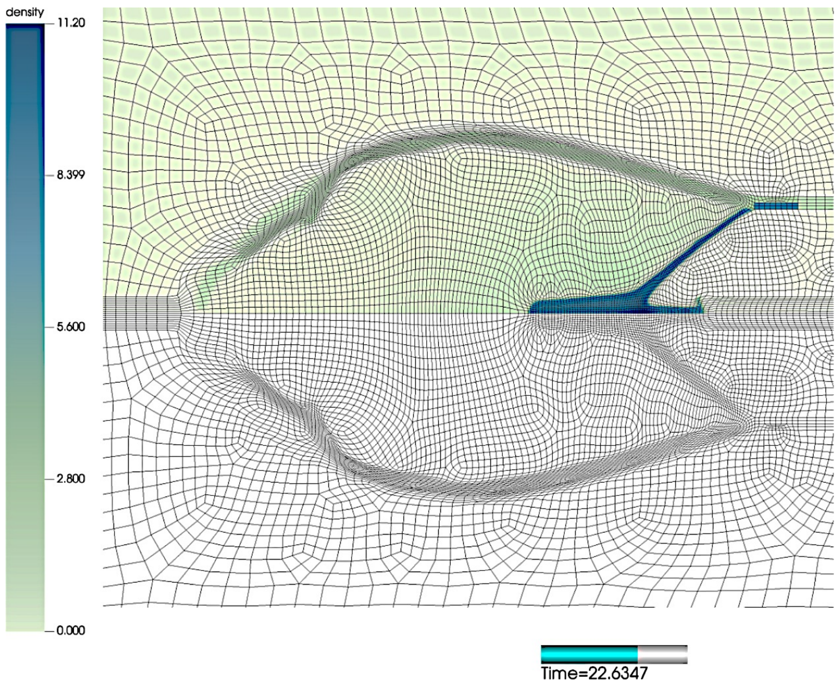
- Match μ_{304}+size:

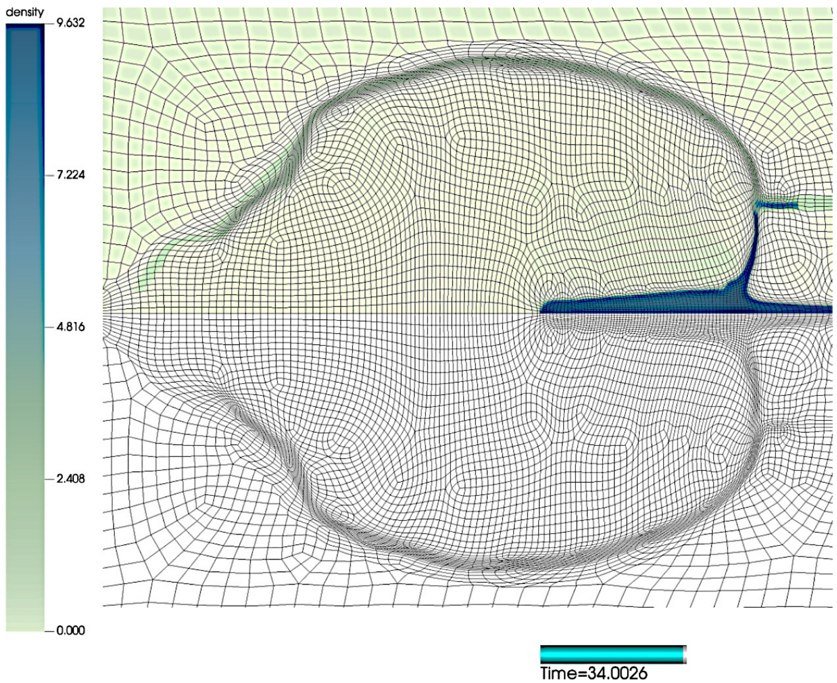
Cases	μ_{304}	μ_{316}	Compound	μ_{318}	Compound
1, 2, 3	$\frac{1}{v}$	$\frac{1}{2\,v}$	$\mu_{304} + 2\,\mu_{316}$	$\frac{1}{2\,v^2}$	$\mu_{304}^2 + 2\,\mu_{318}$
4, 6	$\frac{v^2}{3\sqrt{3}}$	$\frac{v}{2}$	$\mu_{304} + \left(\frac{4}{3\sqrt{3}}\right)\,\mu_{316}^2$	$\frac{v^2}{2}$	$\mu_{304} + \left(\frac{2}{3\sqrt{3}}\right)\,\mu_{318}$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

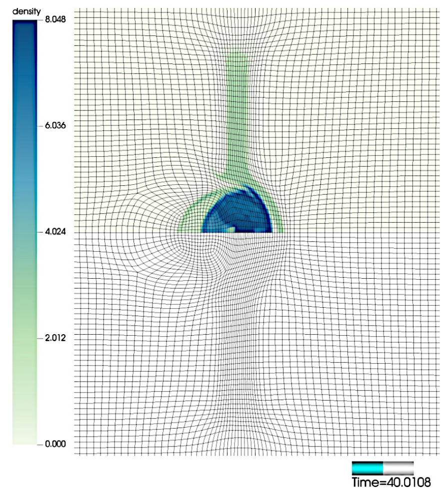
- Computed by μ_{94} with $\lambda = 1.5$ (the default weight)
- Targets 3:1 volume ratio.
- Previously computed by a non-balanced metric, resulting in many trials / errors.

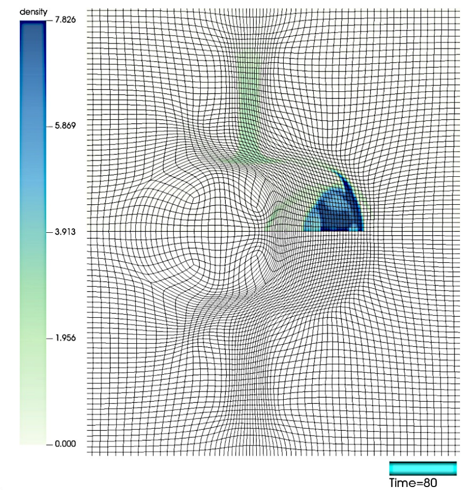




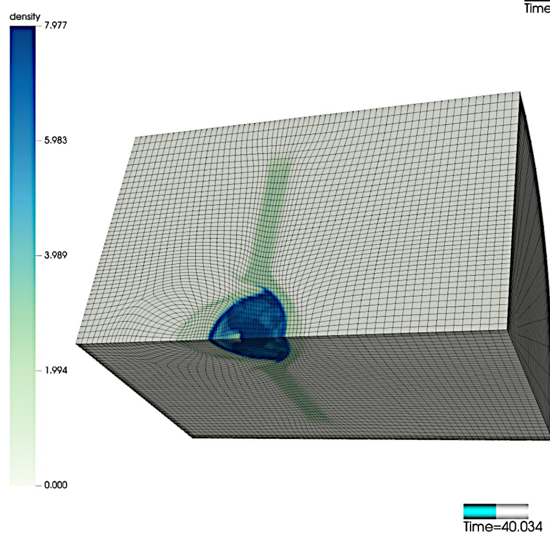
Application results – 2D & 3D ball impact

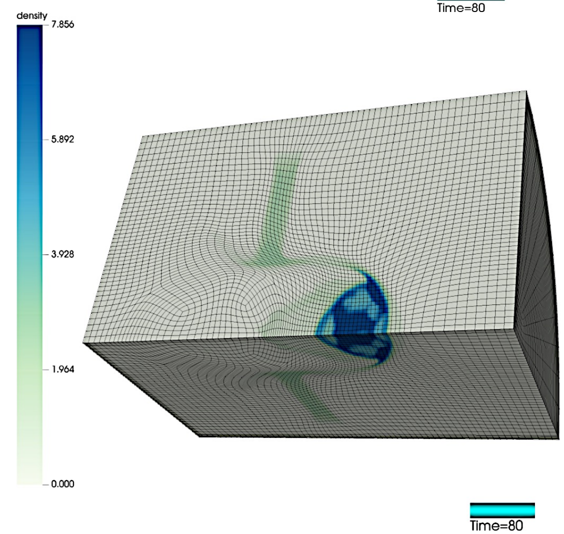
- Computed by μ_{94} with $\lambda = 1.5$ (the default weight)
- Targets 2:1 volume ratio.





- Computed by μ_{338} with $\lambda = 0.1$ * default.
- Puts more emphasis on element shape





Summary

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

$$\mu_{94} = \mu_2 + \lambda\, \mu_{56} \qquad \mu_{338} = \mu_{302} + \lambda\, \mu_{318}$$

$$\mu_{90} = \mu_{50} + \lambda\, \mu_{77} \qquad \mu_{370} = \mu_{301} + \lambda\, \mu_{316}$$

- 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

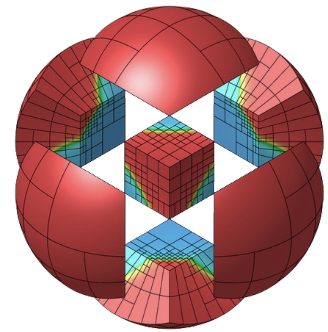
- Arbitrary-order H1, H(curl), H(div)- and L2 elements
- Arbitrary order curvilinear meshes
- MPI scalable to millions of cores + GPU accelerated
- Enables development from laptops to exascale machines.

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

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