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Title: Thirty years at LANL - case study

Author(s): Shashkov, Mikhail Jurievich

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Thirty years at LANL - case study

Mikhail Shashkov
XCP-4, X-Computational Physics Division, LANL

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Time Line

- Started to work at LANL - February 1994, T-Division, Long Term Visiting Scientist
- Staff Member, Green Card, April 1997
- ASCR Project on Mimetic Methods 2000-2017
- US Citizenship, 2003, Q Clearance
- Team Leader, 2005
- Scientist 5, 2008
- Editorial Boards:
  - SIAM Journal on Numerical Analysis - 2009-2015
  - Journal of Computational Physics - 2015-2022
- Moved to New X-Computational Physics Division - 2011
- LANL FELLOW - 2012
- SIAM FELLOW - 2014
- Scientis 6 - 2018

Credentials

- PhD - 1979, Keldysh Institute of Applied Mathematics, Moscow, Russia.
- Habilitation - 1991, Moscow State University, Moscow, Russia.
- Research.com: Ranked in Mathematics: US-301, World-581, D-Index-55
- Google Scholar - h-index:59, Citations 12783, 3353 since 2019
- Researchgate.net - h-index:59,Citations:11489, Publications:365
- LANL - Scientist 6 (6), LANL Fellow, SIAM Fellow
- Principal organizer of Multimat Conference 2002, last conference - Zurich 2021, Next Conference, Breckenridge, CO - 2024
- Collaborators: LLNL, SNL, AWE (UK), CEA (France), Germany, Czechia, Italy, Russia
- PDs - 11, many students, several of them now work at LANL

Main Scientific Contributions

- Mimetic finite differences (MFD) - Origin of the Virtual Element Method (VEM)
  - Discrete vector and tensor analysis
  - Discretizations: Diffusion, Maxwell, Lagrangian hydrodynamics on general polyhedral meshes, discontinuous coefficients
  - Important publications:
    - M. Shashkov, Conservative Finite-Difference Methods on General Grids, CRC Press, Boca Raton, Fl, 1996
    - Compatible Spatial Discretizations,Conference Proceedings, 2006 Editors: D. N. Arnold, P. B. Bochev, R. B. Lehoucq, R. A. Nicolaides, M. Shashkov,
    - J. M. Hyman and M. Shashkov, The Orthogonal Decomposition Theorems for Mimetic Finite Difference Methods, SIAM Journal on Numerical Analysis, Volume 36, No. 3, pp. 788–818, (1999).
    - F Brezzi, K Lipnikov, M Shashkov, Convergence of the mimetic finite difference method for diffusion problems on polyhedral meshes SIAM Journal on Numerical Analysis 43 (5), 1872-1896, 2005
    - K Lipnikov, G Manzini, M Shashkov, Mimetic finite difference method Journal of Computational Physics 257, 1163-1227, 2014

Main Scientific Contributions

- Multi-material Arbitrary-Lagrangian-Eulerian Methods

  AJ Barlow, PH Maire, WJ Rider, RN Rieben, MJ Shashkov Arbitrary LagrangianEulerian methods for modeling high-speed compressible multimaterial flows Journal of Computational Physics 322, 603-665, 2016

  - Multi-material Lagrangian Hydrodynamics
    - Compatible, conservative discretization of polyhedral meshes
      EJ Caramana, DE Burton, MJ Shashkov, PP Whalen The construction of compatible hydrodynamics algorithms utilizing conservation of total energy Journal of Computational Physics 146 (1), 227-262, 1998
    - Tensor Artificial Viscosity
      EJ Caramana, MJ Shashkov, PP Whalen Formulations of artificial viscosity for multi-dimensional shock wave computations Journal of Computational Physics 144 (1), 70-97
      JC Campbell, MJ Shashkov A tensor artificial viscosity using a mimetic finite difference algorithm Journal of Computational Physics 172 (2), 739-765,2001
    - Treatment of parasitic mesh motion
      EJ Caramana, MJ Shashkov Elimination of artificial grid distortion and hourglass-type motions by means of Lagrangian subzonal masses and pressures Journal of Computational Physics 142 (2), 521-561
    - Isogeometric analysis
      Y Bazilevs, I Akkerman, DJ Benson, G Scovazzi, MJ Shashkov Isogeometric analysis of Lagrangian hydrodynamics Journal of Computational Physics 243, 224-243, 2013
    - Closure models for multi-material cells
      A Barlow, R Hill, M Shashkov Constrained optimization framework for interface-aware sub-scale dynamics closure model for multimaterial cells in Lagrangian and arbitrary LagrangianEulerian hydrodynamics Journal of Computational Physics 276, 92-135, 2014
      A Barlow, M Klima, M Shashkov Constrained optimization framework for interface-aware sub-scale dynamics models for voids closure in Lagrangian hydrodynamics Journal of computational physics 371 914-944, 2018
      An interface-aware sub-scale dynamics multi-material cell model for solids with void closure and opening at all speeds M Klima, A Barlow, M Kucharik, M Shashkov Computers & fluids 208, 10457, 2020

Main Scientific Contributions

- Rezone - mesh improvement
  JM Hyman, S Li, P Knupp, M Shashkov An algorithm for aligning a quadrilateral grid with internal boundaries Journal of Computational Physics 163 (1), 133-149, 2000
  P Knupp, LG Margolin, M Shashkov Reference Jacobian optimization-based rezone strategies for arbitrary Lagrangian Eulerian methods Journal of Computational Physics 176 (1), 93-128, 2002
  RV Garimella, MJ Shashkov, PM Knupp Triangular and quadrilateral surface mesh quality optimization using local parametrization Computer Methods in Applied Mechanics and Engineering 193 (9-11), 913-928,2004

  M Berndt, M Kucharik, MJ Shashkov Using the feasible set method for rezoning in ALE

  Procedia Computer Science 1 (1), 1885-1892, 2010

Main Scientific Contributions

- Remap - Constrained Data Transfer Between Meshes

LG Margolin, M Shashkov Second-order sign-preserving conservative interpolation (remapping) on general grids Journal of Computational Physics 184 (1), 266-298,2003
R Loubere, MJ Shashkov A subcell remapping method on staggered polygonal grids for arbitrary-LagrangianEulerian methods Journal of Computational Physics 209 (1), 105-138, 2005
M Kucharik, M Shashkov, B Wendroff An efficient linearity-and-bound-preserving remapping method Journal of computational physics 188 (2), 462-471, 2003
M Kucharik, M Shashkov, B Wendroff An efficient linearity-and-bound-preserving remapping method Journal of computational physics 188 (2), 462-471, 2014
R Garimella, M Kucharik, M Shashkov An efficient linearity and bound preserving conservative interpolation (remapping) on polyhedral meshes Computers & fluids 36 (2), 224-237, 2007
R Garimella, M Kucharik, M Shashkov An efficient linearity and bound preserving conservative interpolation (remapping) on polyhedral meshes Computers & fluids 36 (2), 224-237, 2010
P Bochev, D Ridzal, G Scovazzi, M Shashkov Formulation, analysis and numerical study of an optimization-based conservative interpolation (remap) of scalar fields for arbitrary LagrangianEulerian methods Journal of Computational Physics 230 (13), 5199-5225, 2011
P Bochev, M Shashkov Constrained interpolation (remap) of divergence-free fields Computer methods in applied mechanics and engineering 194 (2-5), 511-530, 2005
M Kucharik, M Shashkov Extension of efficient, sweptintegrationbased conservative remapping method for meshes with changing connectivity International journal for numerical methods in fluids 56 (8), 1359-1365, 2008
M Klma, M Kuchak, J Velechovsk, M Shashkov Second-invariant-preserving Remap of the 2D deviatoric stress tensor in ALE methods Computers & Mathematics with Applications 78 (2), 654-669, 2019

M Kenamond, D Kuzmin, M Shashkov Intersection-distribution-based remapping between arbitrary meshes for

staggered multi-material arbitrary Lagrangian-Eulerian hydrodynamics Journal of Computational Physics 429,

110014, 2021

Main Scientific Contributions

- Reconnection-based ALE

R Loubere, PH Maire, M Shashkov, J Breil, S Galera ReALE: A reconnection-based arbitrary-LagrangianEulerian method Journal of Computational Physics 229 (12), 4724-4761, 2010
J Breil, T Harribey, PH Maire, M Shashkov A multi-material ReALE method with MOF interface reconstruction Computers & Fluids 83, 115-125, 2013
W Bo, M Shashkov R-adaptive reconnection-based arbitrary Lagrangian Eulerian method-R-ReALE J. Math. Study 48 (2), 125-167, 2015
W Bo, M Shashkov Adaptive reconnection-based arbitrary Lagrangian Eulerian method Journal of Computational Physics 299, 902-939, 2015
2D & 3D voronoi meshes generation with ShaPo J Pouderoux, M Charest, M Kenamond, M Shashkov The 8th international conference on numerical methods for multi-material fluid flow (MULTIMAT 2017) , 2017

Moments-based interface reconstruction -time line

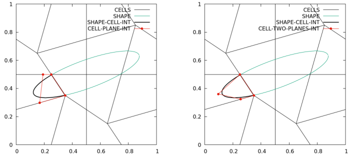
- V. Dyadechko, M.J. Shashkov Moment-of-Fluid interface reconstruction Tech. Rep. LA-UR-05-7571 Los Alamos National Laboratory, Los Alamos (2005)
- V. Dyadechko, M.J. Shashkov Reconstruction of multi-material interfaces from moment data J. Comput. Phys., 227 (2008), pp. 5361-5384
- H.T. Ahn, M. Shashkov Multi-material interface reconstruction on generalized polyhedral meshes J. Comput. Phys., 226 (2007), pp. 2096-2132
- H.-T. Ahn, M. Shashkov Geometric algorithms for 3D interface reconstruction M.L. Brewer, David Marcum (Eds.), Proceedings of the 16th International Meshing Roundtable, Springer, Berlin Heidelberg (2008), pp. 405-422
- M. Shashkov, E. Kikinzon, Moments-based interface reconstruction, remap and advection, JCP (479), 111998, 2023
- M. Shashkov Adaptive moments-based interface reconstruction, Journal of Computational Physics Volume 494, 1 December 2023, 112504

Outline

- Different perspective on interface reconstruction
- Moments-based interface reconstruction - moment of fluid (MOF), MOF^2
- Moments and their meaning, reference ellipse
- Examples of reconstruction in one cell
- Interface reconstruction on full mesh
- Advection
- Interface remapping
- Arbitrary Lagrangian-Eulerian Methods - Sketch
- Possible Extensions.
- Conclusion and Future Work

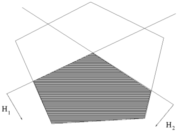
Different Perspective on Interface Reconstruction

- Standard point of view on interface reconstruction - approximate interface in each cell of the mesh - approximation of the fragment of the curve
  - Piece-wise linear construction (PLIC), circles, parabolas, multi-lines - uses information about volume fractions from neighboring cells

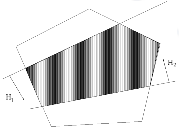


- New Perspective - Material Region Intersects with cells - in each cell there is fragment of the material - FOM - representing material in this cell
  - Main characteristics of FOM are moments - Approximate FOM
  - Intersect cell with half-plane - Moment of Fluid -MOF^1_{1hp} - uses zero and first moments - formally PLIC
  - Intersect cell with two half-planes - MOF^2_{2hp} - uses zero, first and second moments

MOF^2_{2hp} -Exactly reproducible interface configurations

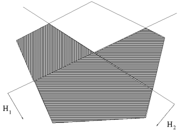


Corner

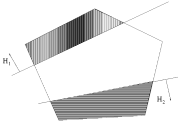


Stripe-filament

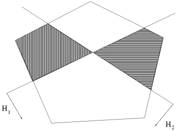
One polygon



Inverted corner



Disconnected Pieces



Bow-tie

Two polygons

Moments of a region and their meaning

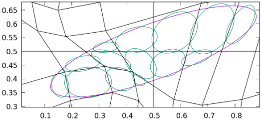
- Raw-geometric moments - $M_{kl}(\Omega_{mat}) = \int_{\Omega_{mat}} x^k\, y^l dV$,
- Zero moment - area $M_{00}(\Omega_{mat}) = \int_{\Omega_{mat}} 1\, dxdy$.
- Ratio -first moments and the zeroth moment - centroid - location

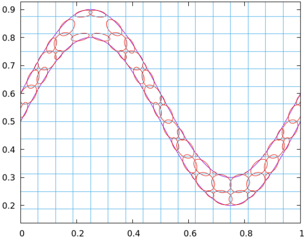
$$(x^c, y^c) = \left(\frac{M_{10}}{M_{00}}, \frac{M_{01}}{M_{00}}\right) = \left(\frac{\int_{\Omega_{mat}} x\, dxdy}{\int_{\Omega_{mat}} 1\, dxdy}, \frac{\int_{\Omega_{mat}} y\, dxdy}{\int_{\Omega_{mat}} 1\, dxdy}\right).$$

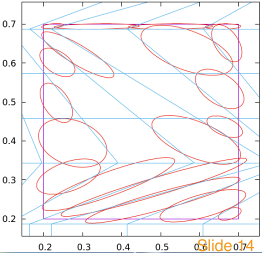
- Second moments allows to construct ellipse (ellipsoid) - characterize orientation main axes and elongations along those axes
  - Scaled central second moments - $\mu'_{kl}(\Omega_{mat}) = \int_{\Omega_{mat}} (x - x^c_{\Omega_{mat}})^k\, (y - y^c_{\Omega_{mat}})^l\, dxdy \Big/ M_{00}$
  - Covariance matrix - $\begin{bmatrix} \mu'_{20} & \mu'_{11} \\ \mu'_{11} & \mu'_{02} \end{bmatrix}$ - symmetric semi-definite

Reference Ellipses

- Eigenvectors of covariance matrix give directions of the main axes of ellipse
- Eigenvalues are proportional to lengths of main axes
- Using zero, first and second moments one can reconstruct unique ellipse, which center coincides with centroid of shape and which area is equal to area of shape







MOF^2_{2hp} Algorithm - Some Details

- Objective function - Many Options - Dimensionless

$$F(\alpha_1,d_1;\alpha_2,d_2)=\sum_{k,l:2\geq k+l\geq 1}\left(\frac{M^{act}_{k,l}}{(M^{act}_{00})^{1+\frac{k+l}{2}}}-\frac{M^{ref}_{k,l}}{(M^{ref}_{00})^{1+\frac{k+l}{2}}}\right)^2 .$$

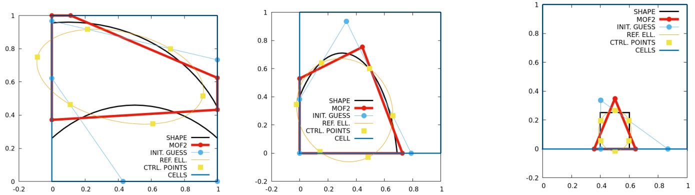
- Constrained (area-zero moment) non-linear least squares optimization

$$\arg\min_{(\alpha_1,d_1),(\alpha_2,d_2):M_{00}=M^{ref}_{00}} F(\alpha_1,d_1,\alpha_2,d_2) .$$

- Computation of Objective Function
  - Parameters $(\alpha_1, d_1, \alpha_2, d_2)$ define two half-planes
  - Intersect half-planes with cell - produces one or two polygons
  - Compute actual moments of the resulting polygon(s), compute objective function

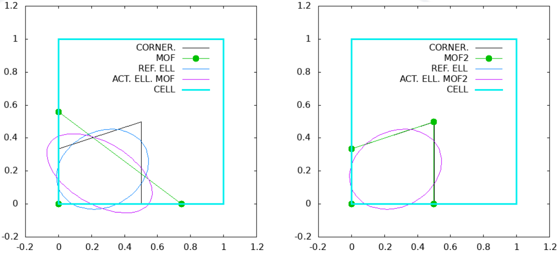
MOF^2_{2hp} Algorithm - Some Details

- Optimization software - NLPQLP - sequential quadratic programming algorithm with distributed and non-monotone line search.
- Translation and scaling of cell - linear transformation - to reference space
- Initial guess - half-planes defined by chords of reference ellipse



- Area fix - compensate for inaccuracy of optimization software
- Inverse linear transformation to physical space

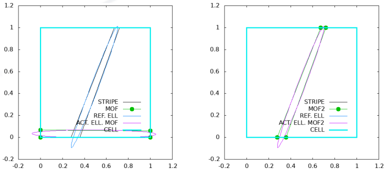
One cell examples



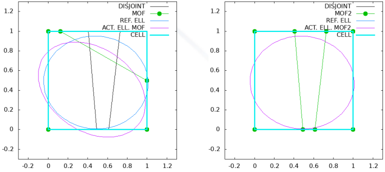
MET.	MOF	MOF^2
M_{00}	6.343E-012	2.083E-013
M_{10}	3.848E-003	2.633E-011
M_{01}	5.120E-003	4.409E-012
M_{20}	1.529E-004	1.537E-011
M_{11}	5.208E-003	7.273E-012
M_{02}	1.665E-003	1.254E-012
SD	9.214E-002	7.639E-010

Corner

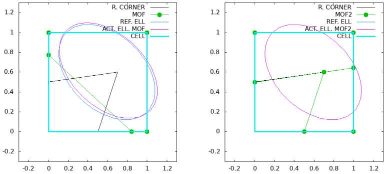
One cell examples



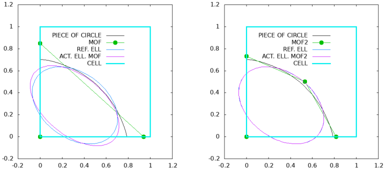
Stripe - Filament



Disjoint pieces - Compliment to Filament



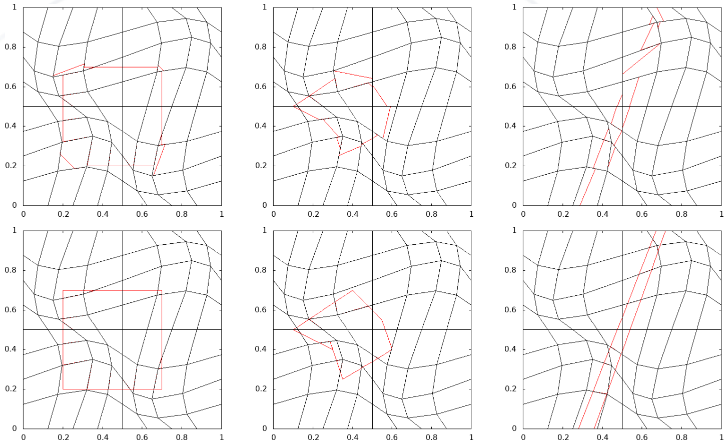
Re-entrant corner



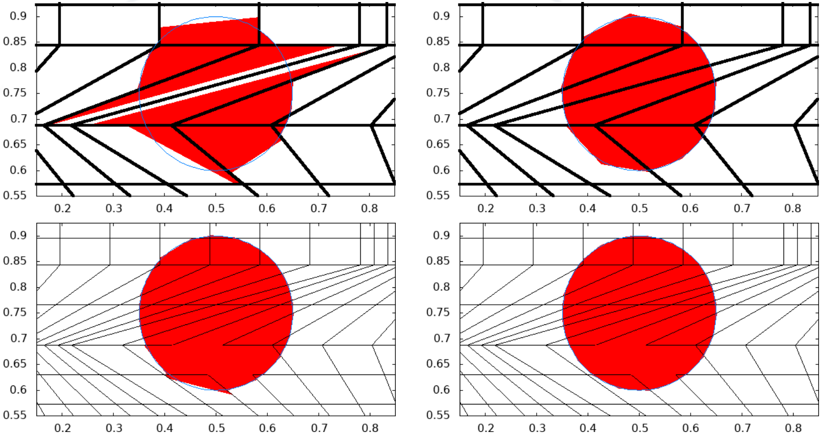
Piece of Circle

Interface Reconstruction on Full Mesh

Exactly Reproducible Shapes - Polygons

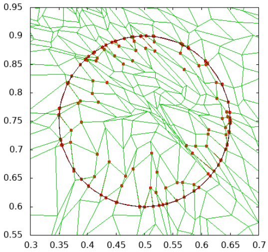


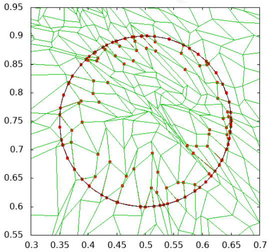
Interface Reconstruction on Full Mesh - Circle - Kershaw Mesh



MOF^1_{1hp} MOF^2_{2hp}

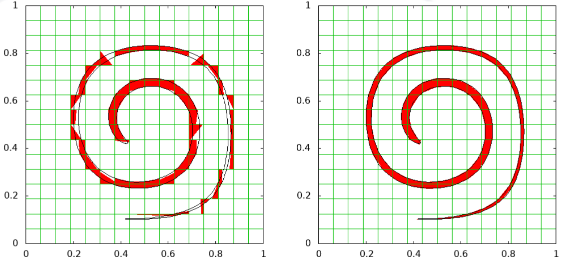
Interface Reconstruction on Full Mesh - Circle - Shestakov Mesh





METH.	M10	M01	M20	M11	M02	SD	SD-MAX
MOF^1_{1hp}	2.529E-008	4.022E-008	2.289E-008	4.081E-008	6.674E-008	1.871E-004	3.114E-005
MOF^2_{2hp}	4.504E-009	6.912E-009	7.026E-009	5.853E-009	9.455E-009	8.191E-005	1.534E-005

Interface Reconstruction on Full Mesh - Convergence Study - Swirl

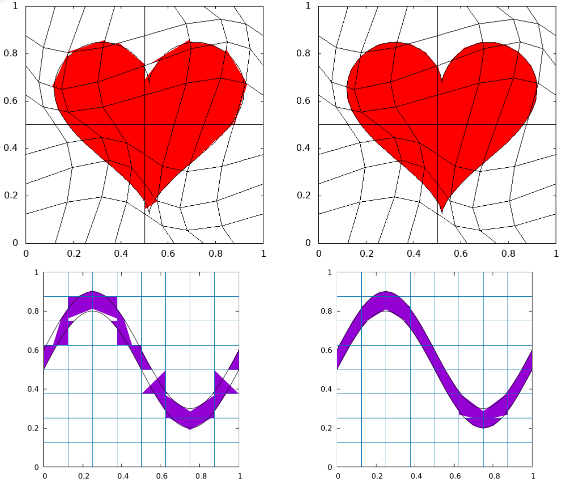


MOF^1_{1hp}	M10	M01	M20	M11	M02	SD	SD-MAX
17 $\times$ 17	3.263E-004	1.991E-004	3.718E-004	1.895E-004	2.105E-004	3.643E-002	1.930E-003
32 $\times$ 32	2.975E-005	3.352E-005	4.436E-005	2.276E-005	2.685E-005	7.961E-003	4.665E-004

MOF^2_{2hp}	M10	M01	M20	M11	M02	SD	SD-MAX
17 $\times$ 17	2.136E-005	1.107E-005	2.219E-005	1.295E-005	1.198E-005	3.696E-003	2.174E-004
32 $\times$ 32	9.981E-007	7.781E-007	1.266E-006	6.429E-007	8.051E-007	5.999E-004	2.924E-005

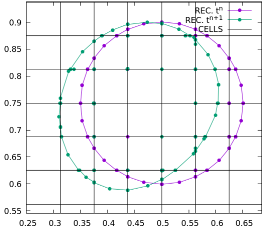
Interface Reconstruction on Full Mesh - Examples - New Shapes

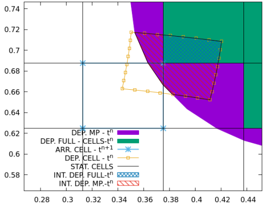
Heart, Snake

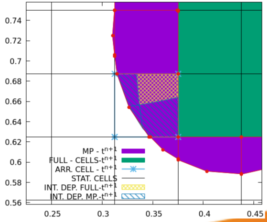


Advection

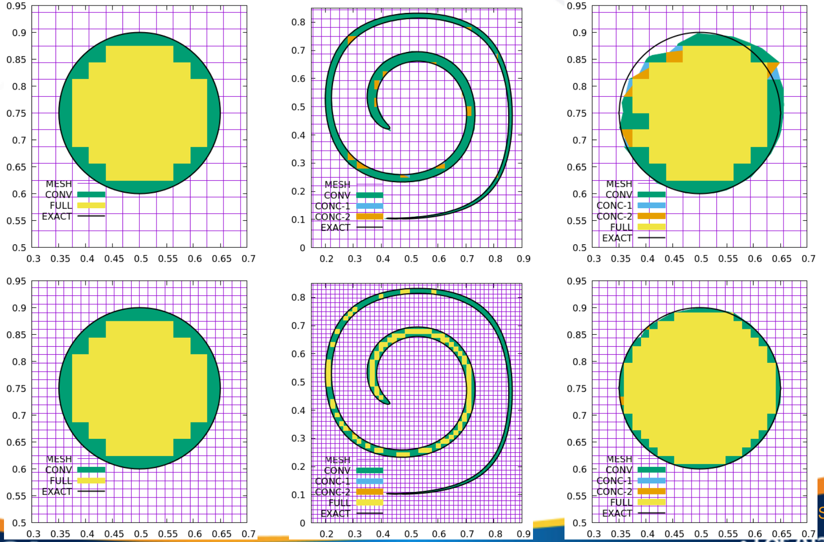
1. Backtracking of the vertices of the arrival cells (using RK4) and forming departure cells (polygons) by connecting the backtracked points by straight lines.
2. Intersection of the departure cells with the full cells and material polygons on the stationary mesh at t^n . It produces several intersection polygons that contain the material.
3. Forward-tracking (using RK4) of the intersection polygons.
4. Computation of moments of forward-tracked intersection polygons and aggregation of those moments - the results serve as the reference moments for the MOF[2] algorithm.



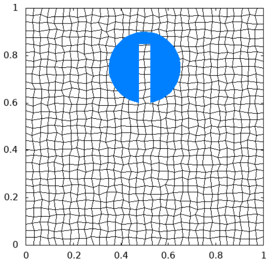


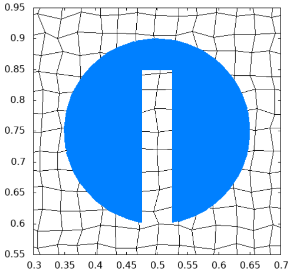


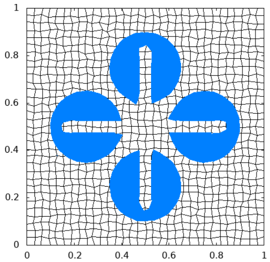
Advection - Swirl



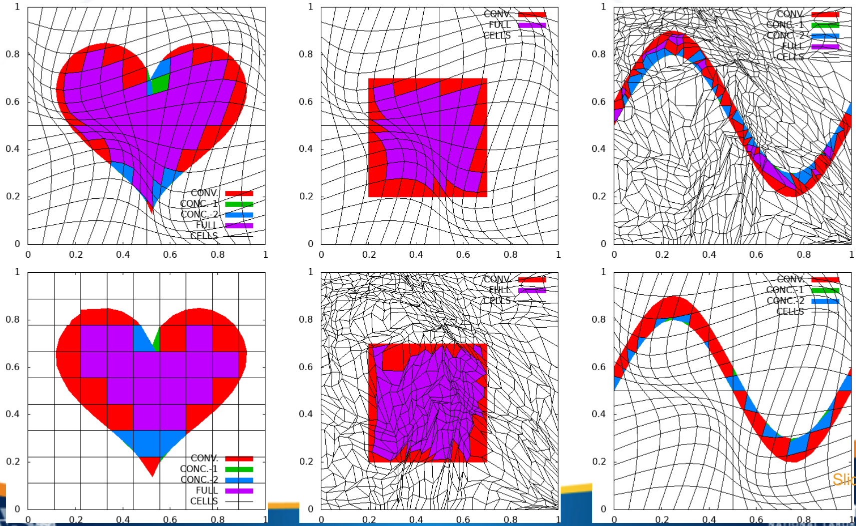
Advection - Arbitrary Mesh - Zalesak's Notched Disk





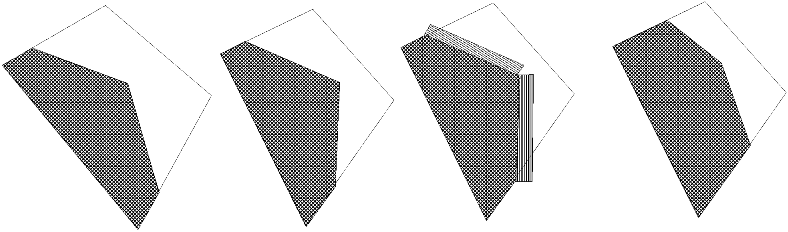


Remap of Material Polygons



Multimaterial Arbitrary Lagrangian-Eulerian Methods - Sketch

- Lagrangian stage - solution and the computational mesh are updated;
- Rezoning stage - nodes of the Lagrangian mesh are moved to improve its quality;
- Remapping stage - Lagrangian solution is transferred to the optimized mesh.



Mesh t^n Lag. mesh t^{n+1} Sub. Dynam. MOF[2] Rec.

Conclusion

- New MOF^2_{2hp} Interface reconstruction method
  - Uses zero, first and second moments
  - Does not require information from neighboring cells
  - Exactly reproduces corners, filaments and their compliments
- Moments-based Advection, Remap, ALE
- References
  - Moments-based interface reconstruction, remap and advection, M. Shashkov, E. Kikinzon, JCP (479), 111998, 2023
  - https://www.researchgate.net/publication/362606507
  - Adaptive moments-based interface reconstruction, M. Shashkov, Journal of Computational Physics Volume 494, 1 December 2023, 112504
- Authors would like to thank H.T. Ahn, V. Dyadechko, M. Sussman, R. Giddings, R. Scardovelli, M. Kucharik, D. Ridzal, B. Rider, S. Tokareva, O. Desjardins, N. Carlson, M. Berndt, P. Vachal, M. Francois, A. Barlow, P.-H. Maire, R. Loubere, R. Hill, R. Chiodi, R. Garimella, S. Schofield T. Maric, D. Kothe, J. Yao, K. Joy, E. Kikinzon for many fruitful discussions over the years.