LA-UR-16-20607

Approved for public release; distribution is unlimited.

Title: Adaptive Reconnection-based Arbitrary Lagrangian Eulerian Method

Author(s): Shashkov, Mikhail Jurievich
Bo, Wurigen

Intended for: Presentation at LLNL, operational visit

Issued: 2016-02-03

Disclaimer:

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Adaptive Reconnection-based Arbitrary Lagrangian Eulerian Method **A-ReALE**

Mikhail Shashkov, XCP-4, XCP Division, LANL

Wurigen Bo, CCS-2, CCS Division, LANL

Currently in EXA Corporation

Thanks to

S. Sambasivan, S. Diot and S. Mao

R. Loubere, J. Breil, S. Galera, P.-H. Maire, A. Barlow, G. Ball

Outline

- ReALE
- Adaptive Reconnection-based ALE - A-ReALE
 - A-ReALE Concept
 - Monitor Function, Equidistribution Principle
 - Main tool: Weighted-centroidal Voronoi Tessellation
 - Adaptations strategies: Maintaining spatial resolution
 - How to construct weighted-centroidal Voronoi Tessellation?
 - How to Compare ReALE and A-ReALE Methods?
 - Numerical Examples, Sedov, triple point, shock-cavity interaction
- Conclusion and Future Work

Standard Reconnection-based Arbitrary Lagrangian-Eulerian ReALE Methods

- Lagrangian Phase — General polygonal meshes
- Rezone Phase
 - Allows mesh reconnection —
 - Voronoi Meshes
 - Mesh Smoothing - Centroidal Voronoi
 - Number of Cell does not change
- Remap Phase
 - Remapping between polygonal meshes with different connectivity
 - Intersection-based Remap

Adaptive Reconnection-based Arbitrary Lagrangian-Eulerian A-ReALE Methods

- Lagrangian Phase — General polygonal meshes
- Rezone Phase
 - Add/Remove Cells - Monitor, Equidistribution, Weighted-centroidal Voronoi
 - Mesh Reconnection - Voronoi
 - Number of Cells **May Change**
- Remap Phase
 - Remapping between polygonal meshes with different connectivity and different number of cells
 - Intersection-based Remap

Experiment

Standard ReALE

A-ReALE

Shock over Cavity

Adaptation - Design Principles

- **Monitor Function** $\varphi(\mathbf{x}, t) > 0$
Problem Dependent and Goal Oriented
 - Interpolation Error, Error Estimation
 - Feature Resolution - shock, contact, interface, boundary-layer
- **Equidistribution Principle** - $\int_{\Omega_i} \varphi(\mathbf{x}, t) dV = E(t)$ - **Equidistribution Level**
- **Adaptation strategies**
 - Fixed number of generators - adapting to monitor using equidistribution principle
 - Maintaining constant equidistribution level during the calculation $E(t) = E(t_0) = \text{const}$ - number of generators changes
 - Maintaining given spatial resolution where monitor reaches its max values - number of generators changes
- **Main Tool - Weighted Centroidal Voronoi Meshes**

Monitor Function

- **Raw Monitor** - Interpolation error: $\varphi = \sqrt{\max(|\lambda_1|, |\lambda_2|)}$
 Hessian $H_u = \begin{pmatrix} \partial^2 u / \partial x^2 & \partial^2 u / \partial x \partial y \\ \partial^2 u / \partial x \partial y & \partial^2 u / \partial y^2 \end{pmatrix} = Q^T \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} Q$
- **Smoothing** - smoothing and removing noise
- **Shape Preserving Scaling** - increase min and decreases max values - to avoid very small cells - dt ; and very big cells - accuracy

Sod problem

Raw Monitor

Raw & Smoothed

Smoothed & Scaled

Equidistribution Principle

- **Equidistribution Principle**
 - Computational domain Ω ; Monitor function $\varphi(\mathbf{x})$
 - Mesh with cells Ω_i satisfies equidistribution principle if
$$\int_{\Omega_i} \varphi(\mathbf{x}) dV = \text{const} = E \rightarrow \varphi_i |\Omega_i| \approx E$$
 - Large φ_i - small $|\Omega_i|$
- **How to** construct mesh which satisfies equidistribution principle?
 - **Weighted centroidal Voronoi tessellation**

Voronoi, Weighted-Centroidal Voronoi

Set of generators: $\mathbf{g}_i = (x_i, y_i)$

Voronoi cell: $\Omega_i = \{\mathbf{r} = (x, y) : |\mathbf{r} - \mathbf{g}_i| < |\mathbf{r} - \mathbf{g}_j|, \text{ for all } j \neq i\}$

Mass centroid of the cell ($\psi(\mathbf{r}) > 0$ - given weight function)

$$\mathbf{c}_i^\psi = \int_{\Omega_i} \mathbf{r} \psi(\mathbf{r}) d\mathbf{r} / \int_{\Omega_i} \psi(\mathbf{r}) d\mathbf{r},$$

If $\mathbf{g}_i = \mathbf{c}_i^\psi$ - **weighted-centroidal Voronoi** tessellation

Left - Random with weight; Right - weighted-centroidal

Random sampling

Centroidal Voronoi

Weighted-Centroidal Voronoi Tessellation

■ Properties:

- Local uniformity - spherical hexagons - accuracy of discretization
- $\psi(\mathbf{g}_i) h_i^{d+2} \approx \psi(\mathbf{g}_j) h_j^{d+2}$, $h_i = 2 \max_{\mathbf{r} \in \Omega_i} \|\mathbf{g}_i - \mathbf{r}\|$
 d dimension of the space

■ How to construct mesh which satisfies equidistribution principle?

- For $d = 2$ - $\psi(\mathbf{g}_i) h_i^4 \approx \psi(\mathbf{g}_j) h_j^4$
- For weighted centroidal Voronoi tessellation in 2D $|\Omega_i| \sim h_i^2$
- $\sqrt{\psi(\mathbf{g}_i)} |\Omega_i| \approx \sqrt{\psi(\mathbf{g}_j)} |\Omega_j|$
- If we set $\psi = \varphi^2$, then $\varphi(\mathbf{g}_i) |\Omega_i| \approx \varphi(\mathbf{g}_j) |\Omega_j|$ - Approximate Equidistribution

Resolution and Required Number of Generators

- If mesh satisfies equidistribution principle then

$$\varphi(\mathbf{g}_i) |\Omega_i| \approx \varphi(\mathbf{g}_j) |\Omega_j| \approx \left(\int_{\Omega} \varphi dV \right) / N_g = E$$

N_g - number of generators, E - Equid. Level

- If we **want to achieve desired Equid. Level E** in domain Ω then we **need**

$$N_g^E \approx \left(\int_{\Omega} \varphi dV \right) / E$$

generators

Adaptation Strategy - Maintaining Spatial Resolution

- Monitor function depends on space and time - φ_i^n
- For meshes which satisfy equidistribution $\varphi_i^n A_i^n = E^n$ and therefore $\varphi_{max}^n A_{min}^n = E^n$
- If we would like to **maintain** constant spatial **resolution** for in regions where **monitor** has its **maximum** values - $A_{min}^n = A_{min} = \text{const}$, then Equid. Level has to be $E^n = \varphi_{max}^n A_{min}$
- Number of generators need to maintain prescribed spatial resolution A_{min}

$$N^n \approx \int_{\Omega(t)} \varphi(\mathbf{r}, t) d\mathbf{r} / (\varphi_{max}^n A_{min})$$

How to construct weighted-centroidal Voronoi tessellation?

■ Variational formulation

— Functional

$$\mathcal{K}(\{\mathbf{x}_i\}_{i=1}^N) = \sum_{i=1}^N \int_{\Omega_i} \varphi(\mathbf{x}) \|\mathbf{x} - \mathbf{x}_i\|^2 d\mathbf{x},$$

$$\min_{\{\mathbf{x}_i\}_{i=1}^N} \mathcal{K}(\{\mathbf{x}_i\}_{i=1}^N), \text{ subject to } \mathbf{x}_j = \mathbf{G}_j, j = M + 1, \dots, N.$$

where Ω_i are the Voronoi cells corresponding to the $\mathbf{x}_i$.

- A quasi-Newton method, the limited memory Broyden-Fletcher-Goldfarb-Shanno algorithm (L-BFGS). Need to compute Voronoi tessellation on each iteration
- Derivative

$$\frac{\partial \mathcal{K}}{\partial \mathbf{x}_i} = 2(\mathbf{x}_i - \mathbf{G}_i^*) \int_{\Omega_i} \varphi(\mathbf{x}) d\mathbf{x}$$

where $\mathbf{G}_i^*$ is the mass centroid of Ω_i .

How to construct weighted-centroidal Voronoi tessellation?

■ Initial guess - Quadtree approach

- Total # of required generators $\Phi_i = \int_{\Omega_i^L} \phi(\mathbf{x}) d\mathbf{x}$, $N_{total}^{req} = \left\lfloor \left(\sum_{i=1}^{N_L} \Phi_i \right) / E \right\rfloor$
- Number of generators required in subregion $N_{\sigma_k}^{req} = \left\lfloor \left(\sum_{i: G_i \in \sigma_k} \Phi_i \right) / E \right\rfloor$

(a)

(b)

Quad-tree cells and its associated cells. The dots are the centroids of the cells.

(a) a parent quad-tree cell.

(b) The four children of the parent. The bold lines represent the boundaries of the domains associated with the children.

How to construct weighted-centroidal Voronoi tessellation?

Example

Initial guess

"Equidistributed mesh"

Distribution of E_i

The weight function is given by $\varphi(\mathbf{x}) = (1 + 8e^{-\|\mathbf{x}\|^2/0.32})^2$

The desired equi-distribution level $E = 0.00423$, 2856 generators required

How to Compare ReALE and A-ReALE Methods?

- Choose some final time T compute error (comparison can depend on choice of T)
 - Number of time steps can be different for ReALE and A-ReALE
 - Number of cells is changing in A-ReALE
 - Error model - Ch^q ? What is h ? For A-ReALE we can use $h = \sqrt{A_{min}}$; for ReALE we only can choose $N^{-1/2}$ (for given initial mesh). Small parameter has different meaning and we cannot compare convergence rates.
 - Error strongly depends on choice of initial mesh for ReALE
- Our approach - run A-ReALE, compute error and then choose number of generators in ReALE such that error is approximately the same.
 - Compare total number of generators used in “space-time”.
- One can use number of cells in the “equivalent” uniform mesh - mesh in which all cells have the same area equal to A_{min} - $N_{eq} = A/A_{min}$

Sedov Problem - ReALE vs. A-ReALE-Meshes

Meshes for ReALE - 4000 and A-ReALE - $A_{min} = 1.6 \times 10^{-4}$ - the same final L_1 error

Monitor

A-ReALE

ReALE

Sedov Problem - ReALE vs. A-ReALE-Symmetry

ReALE

UNCLASSIFIED

A-ReALE

Sedov Problem - ReALE vs. A-ReALE-Symmetry

A-ReALE - # of gen. ratio of the # number of generators -finest meshes.

ReALE

A-ReALE

L1 density error vs. time - first order convergence - different h

Sedov Problem - ReALE vs. A-ReALE-Convergence

A_{min}	$e(1)$	$q(1)$
1.6e-4	1.92016e-02	
4e-5	1.02941e-02	0.89941
1e-5	5.21725e-03	0.98046

L1 pressure error for A-ReALE

N	$e(1)$	$q(1)$
4000	2.15568e-02	
16000	1.34996e-02	0.675
64000	5.85117e-03	1.206

L1 pressure error for ReALE

Sedov Problem - ReALE vs. A-ReALE-Comparison

	$e(1)$	$N(1)$	$N_{st}(1)$	time steps
ReALE	5.85117e-03	64000	9.73e7	1716
A-ReALE	5.21725e-03	40970	4.43e7	2107

ReALE, 64000 generators

A-ReALE, $A_{min} = 10^{-5}$

Sedov Problem - ReALE vs. A-ReALE-Comparison

ReALE, 64000 generators A-ReALE, $A_{min} = 10^{-5}$

The scatter plot of pressure along the radial direction - high resolution

A_{min}	N_{eq}	$N(1)$	$N_{eq}/N(1)$
1.6e-4	28274	8557	3.3042
4e-5	113096	19151	5.9055
1e-5	452384	40970	11.042

The equivalent number of generators in a uniform mesh

Triple Point Problem - ReALE vs. **A-ReALE**

Approximately the same number number of generators in space-time

$$N_{\text{ReALE}} \approx 34000, A_{\text{min}}^{\text{A-ReALE}} = 5 \times 10^{-5}$$

ReALE - Mesh, $N_g = 33556$

ReALE - IE

A-ReALE - Mesh, $N_g = 24374$

A-ReALE - IE

$t = 3$

Triple Point Problem - ReALE vs. **A-ReALE**

Vortex Resolution

ReALE

A-ReALE

$t = 5$

Interaction between a shock and cavity

The shadowgraph from the experimental results - Igra et al.

ReALE, Mesh - $N = 6051$

A-ReALE, Mesh - $A_{min} = 2 \times 10^{-3}$, $N(420) = 6450$

ReALE, $N = 39593$

A-ReALE, $A_{min} = 1.25 \times 10^{-4}$, $N(420) = 33179$

	$N(420)$	$N_{st}(420)$	time steps
ReALE $N = 39593$	39593	159559790	4030
A-ReALE $A_{min} = 1.25 \times 10^{-4}$	33179	177856789	7086

UNCLASSIFIED

ShaPo-Voronoi Mesh Generator

Contract with Kitware SAS (Lyon, France) - Joachim Pouderoux
LANL - M. Shashkov, M. Kenamond, M. Berndt, B. Jean, D. Herring
ShaPo-2D Main Features

- 2D Voronoi tessellation from a user provided set of generators within a closed domain
- Domain boundary: a polygon that can be
 - Convex
 - Simply connected
 - Non-convex
 - Multiply-connected - with or without holes
- Provides full connectivity of the generated mesh along with other useful information
 - Points, edges & cells connectivity - using winged edges
 - Input boundary edge a mesh edge stands on, new points introduced on a boundary edge, etc.
- Can merge small edges
- Can perform mesh relaxation Centroidal Voronoi
- Mesh export and visualization functions
- Remeshing layer to remesh part of existing mesh

ShaPo, ReALE and FLAG

LANL SETUP Project - B. Jean, D. Herring

Using ReALE in Combination with Lagrangian and ALE Methods

Personal Communication - A.Barlow (AWE) and G.Ball (AWE)

- Predetermined regions with Lagrangian boundaries with ReALE inside
- Dynamically changing regions with Lagrangian boundaries with ReALE inside
- ALE buffer region

ShaPo-3D Development

Conclusion and Future Work

- Developed new adaptive reconnection based framework
- Demonstrated A-ReALE performance on series of examples
- Papers:
 - W. Bo, M. Shashkov, Adaptive reconnection-based arbitrary Lagrangian Eulerian method, J. of Comput. Phys. 299 (2015) 902-939
 - W. Bo, M. Shashkov, R-Adaptive Reconnection-based Arbitrary Lagrangian Eulerian method R-ReALE, J.Math. Study 48(2) (2015) 125-167.
- Implementation in FLAG - ongoing

Thanks

Picture by M. Berndt (LANL) from Kokoman Pojoaque Valley, NM Liquor Store

Papers, Reports: https://www.researchgate.net/profile/Mikhail_Shashkov