Mimetic Finite Difference Methods for Partial Differential Equations

Mikhail Shashkov

T-7, Los Alamos National Laboratory, shashkov@lanl.gov

webpage: cnls.lanl.gov/$\sim$ shashkov

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"Math advances are essential for the exponential performance increases that will drive scientific discovery through computations" — David Brown (Presentation for ASCR Advisory Committee, Washington D.C. February 27, 2007)

Outline

- Mimetic Finite Difference Methods
- History of the Project — Highlights
  - Discrete Calculus
  - Diffusion Equation, Maxwell's Equations
  - Lagrangian, Free-Lagrangian and Arbitrary Lagrangian-Eulerian Hydrodynamics
- Current Research — Highlights
  - Mimetic Discretizations on Generalized (curved faces) Polyhedral Meshes
  - Discrete Maximum Principle
  - Closure Models for Multimaterial ALE Methods
- Outreach
- How do we train the future workforce?
- Conclusion

What are mimetic methods ?

Methods that mimic important properties of underlying geometrical, mathematical and physical models.

- **Geometry (material interfaces)**
- **Conservation Laws (modeling flows with strong shocks)**
- **Symmetry Preservation (inertial confinement fusion program)**
- **Positivity and Monotonicity Preservation (density, pressure, concentration)**
- **Asymptotic Preserving (radiation hydrodynamics), Long-Time Integration**
- **Duality Properties of Differential Operators (Solvers)**

History of the Project

- **Discrete Vector and Tensor Analysis - Discrete Calculus**
  - **Discrete scalar, vector and tensor functions on wide class of grids**
  - **Discrete analogs of differential operators like div, grad, and curl**
  - **Discrete analogs of the theorems of the vector analysis: Gauss', Stokes', orthogonal decomposition (Hodge).**
  - **Most of PDE's are formulated in terms of divergence, gradient and curl.**
  - **Given discrete analogs of these operators one can discretize wide class of PDE's (many continuous results hold in discrete case.)**

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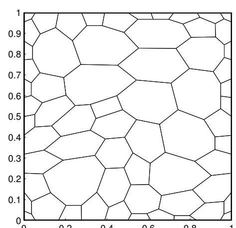
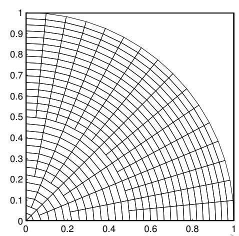
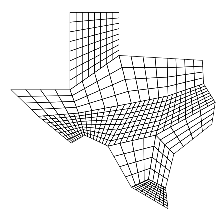
History of the Project

- **Properties of the Mimetic Discretizations for Diffusion Equations**
  - **Complex Three-Dimensional Geometry**
  - **Arbitrary Coordinate Systems (Cylindrical, Spherical)**
  - **Strongly Discontinuous Tensor Conductivity**
  - **Non-Smooth Structured and Unstructured (General Polyhedra), and AMR Meshes**
  - **Symmetric Positive-Definite Linear Systems — Effective Solvers**
  - **Second-order Convergence (New Theory), Accurate Fluxes**
  - **Applications**



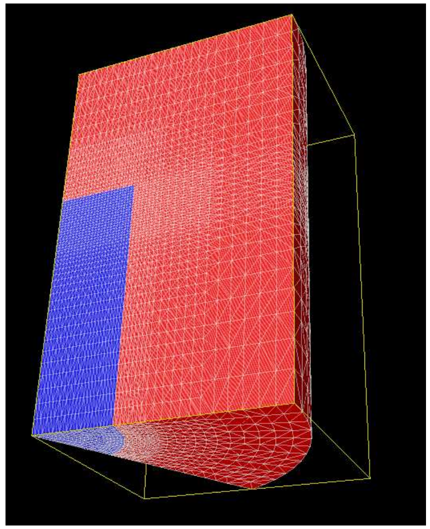


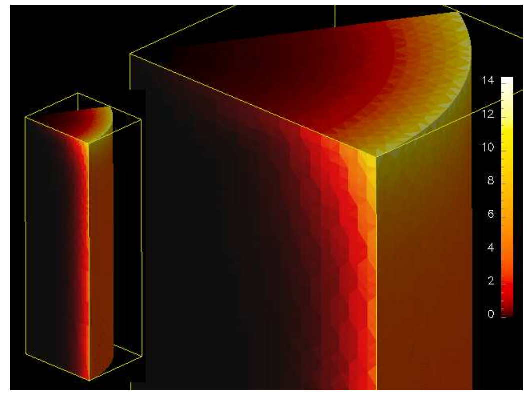


History of the Project

- **Mimetic Discretizations for Maxwell's Equations**
  - **Complex Three-Dimensional Geometry**
  - **Strongly Discontinuous Tensor Permitivity and Permeability.**
  - **Non-Smooth Structured and Unstructured Grids**
  - **Free of Spurious Solutions, Divergence-Free Conditions are Satisfied Exactly**
  - **Stable, Second-Order Convergence, Accurate Electric and Magnetic Fields**

Optimization of the gravity-pour casting processes





The computational domain and grid (200K tets); the blue region is the graphite cylinder, and the red region is free space - left.

The average of the Joule heat in the graphite cylinder over a cycle of the external field; this is the effective heat source that is used to model the heat conduction - right.

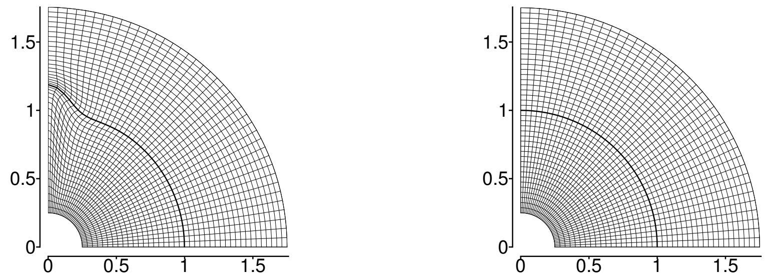
History of the Project

- **Lagrangian, Free-Lagrangian and Arbitrary Lagrangian-Eulerian Hydrodynamics**
  - **Conservative finite-difference methods in 3D and on unstructured grids**
  - **New advanced artificial viscosity for multi-dimensional shock-wave computations**
  - **Elimination of unphysical grid motions (hourglass, artificial vorticity) due to Artificial Null Spaces of the discrete operators**

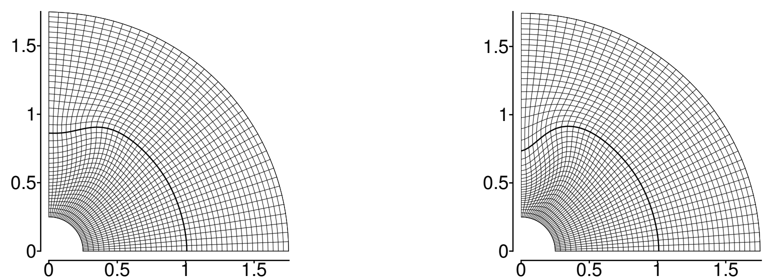
$$\mathbf{DIV}\,\mathbf{A} = 0 \not\leftrightarrow \mathbf{A} = \mathbf{CURL}\,\mathbf{B}\,, \quad \mathbf{GRAD}\,p = 0 \not\leftrightarrow p = const$$

  - **Symmetry (geometrical) preserving methods**

Lagrangian Hydrodynamics — Spatial Symmetries and Curvilinear Meshes — (r, z) Geometry



Symmetric Flow



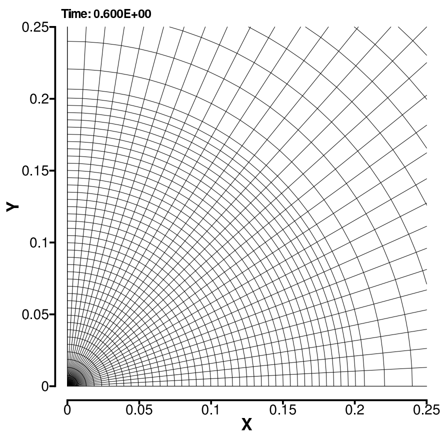
Spherical Rayleigh-Taylor Instability

Standard Method (linear edges) **Curvilinear Meshes**

Lagrangian Hydrodynamics — Artificial Viscosity

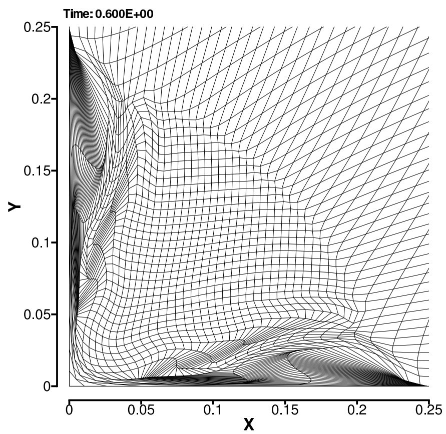
Artificial Viscosity is Required for Simulations of Shocks

Mesh for Noh Problem at $t = 0.6$



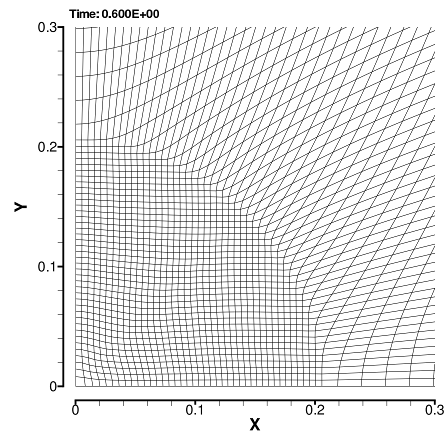
Initial Polar Mesh

Edge Viscosity



Initial Square Mesh

Edge Viscosity



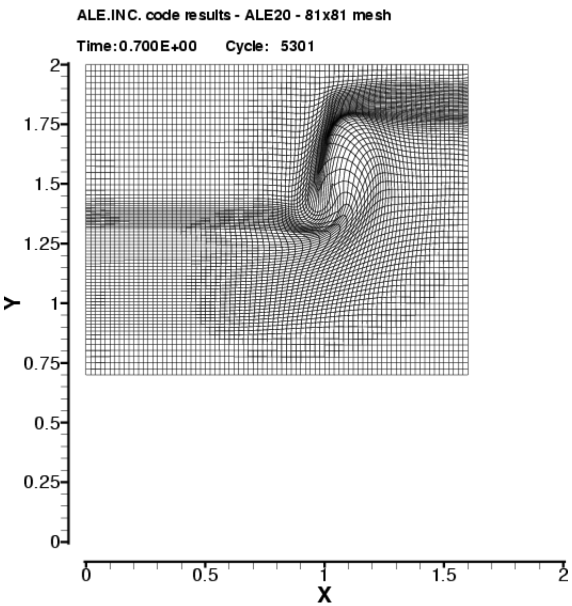
Initial Square Mesh

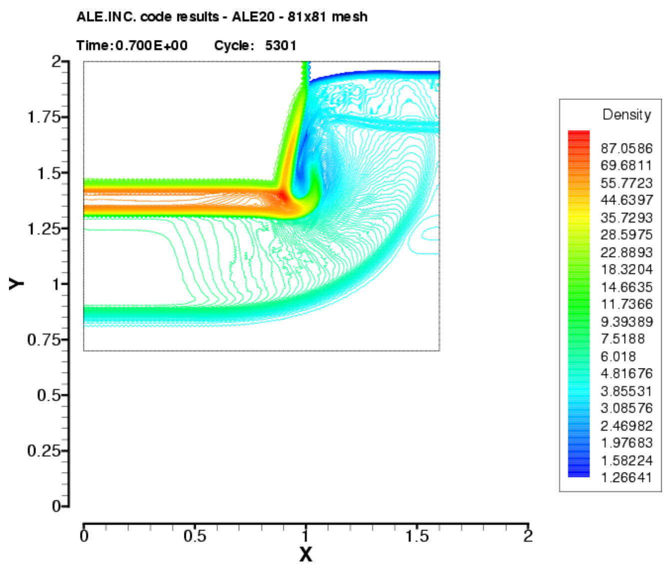
Mimetic Tensor Viscosity

Arbitrary Lagrangian-Eulerian (ALE) Methods

ALE Methods – grid movement is arbitrary and can be used to improve robustness and accuracy

Three Main Stages: Lagrangian, Rezone, Remap





Interaction of Shock with heavy obstacle - ALE INC.(ubator)

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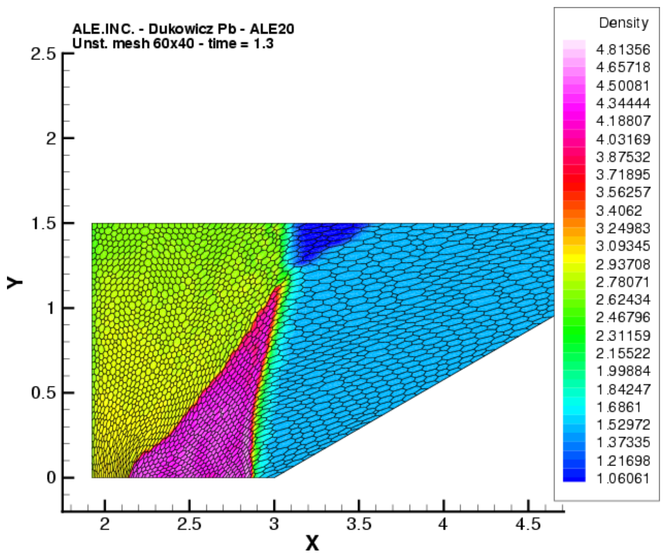
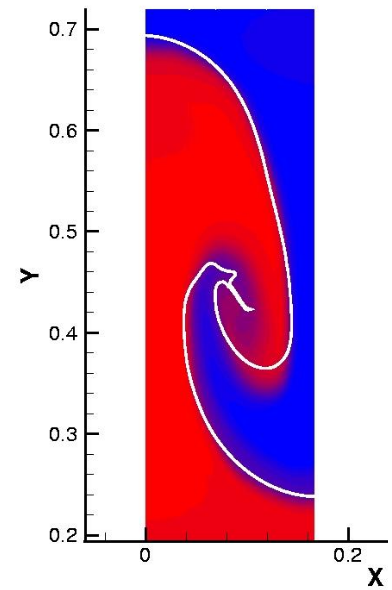
Arbitrary Lagrangian-Eulerian Methods

Examples of ALE INC. Calculations



Shock Refraction Problem

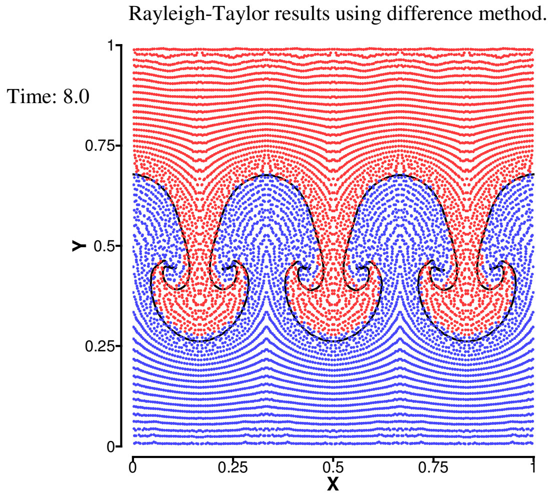
polygonal meshes

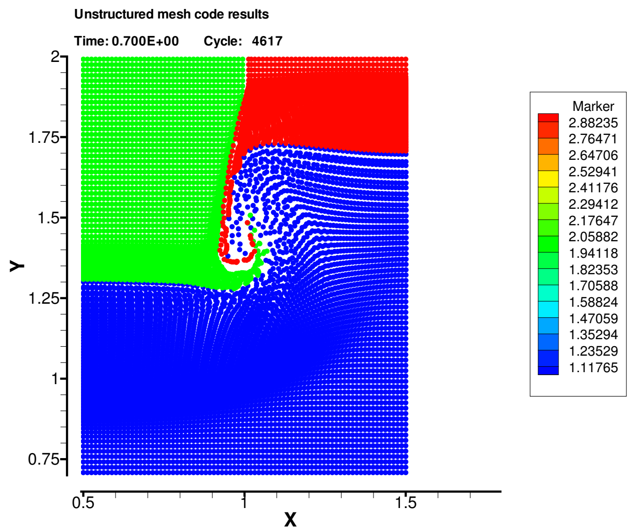


Rayleigh-Taylor Instability

Free-Lagrangian Methods

- Media is represented by set of points, with fixed in time mass.
- Points (Particles) are moving with material
- Connectivity between these points is not fixed, but varies with time — Voronoi tessellation
- Stencil used in discretization is defined by connectivity.





Current Research Highlights

- Mimetic Finite Difference Method - Diffusion Equation - Generalized (Curved Faces) Polyhedral Meshes
- Discrete Maximum Principle
- Multimaterial Arbitrary Lagrangian-Eulerian Methods

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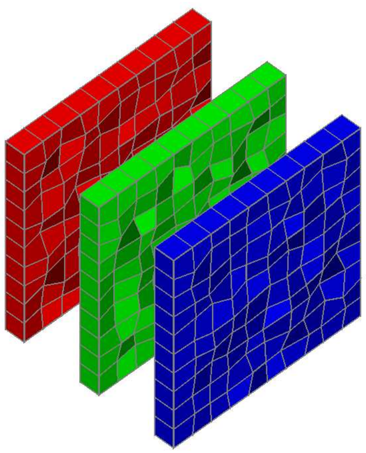
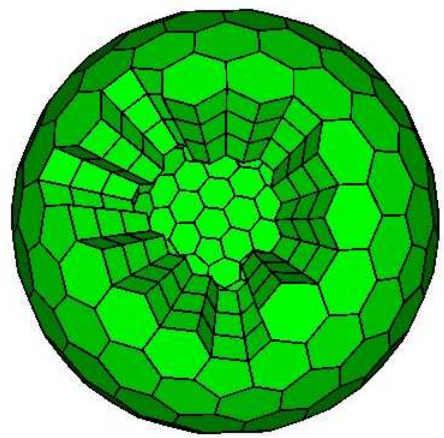
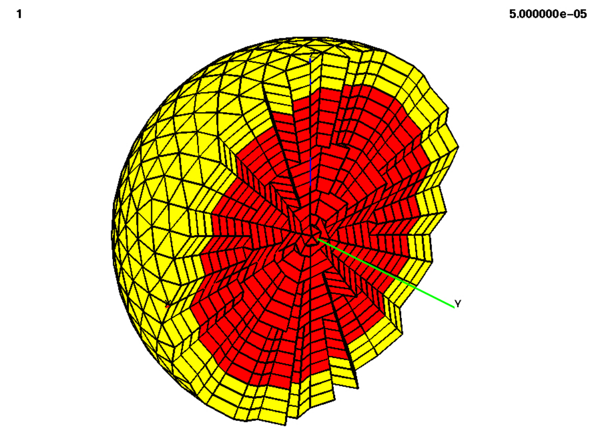
Mimetic Finite Difference Method - Diffusion Equation - Generalized Polyhedral Meshes

$$\mathcal{DIV}\boldsymbol{u}^h = \boldsymbol{Q}^h, \qquad \boldsymbol{u}^h = -\mathcal{GRAD}\boldsymbol{p}^h.$$







- **The MFD method is locally conservative, 2nd-order accurate for $\boldsymbol{p}^h$ and at least 1st-order accurate for $\boldsymbol{u}^h$ on** *generalized (curvilinear faces)* **polyhedral meshes (including AMR meshes). Its practical implementation is surprisingly simple.**

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Key elements of new methodology

- The **patch test** for element E with faces f_i:

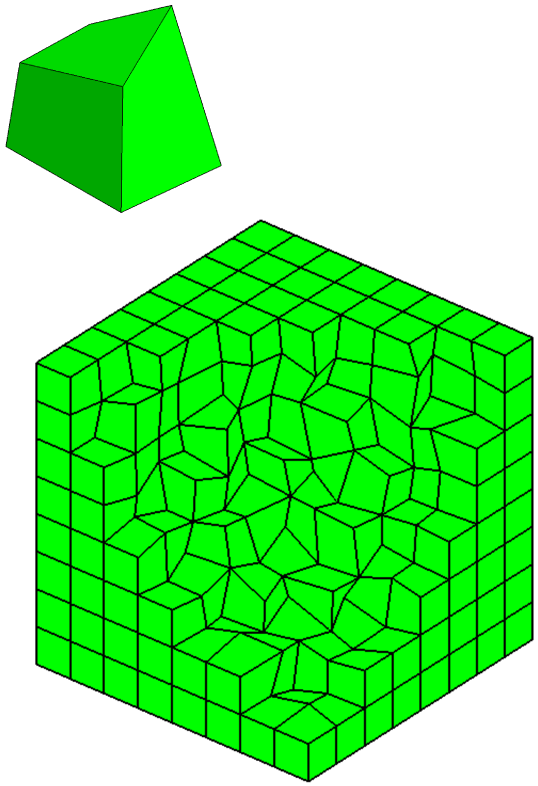
$$[(K\nabla p^1)^h,\, G^h]_E \equiv \int_E p^1 (\mathrm{DIV}\, G^h)_E \mathrm{d}V - \int_{\partial E} p^1 G^h \cdot \vec{n}\, \mathrm{d}S$$

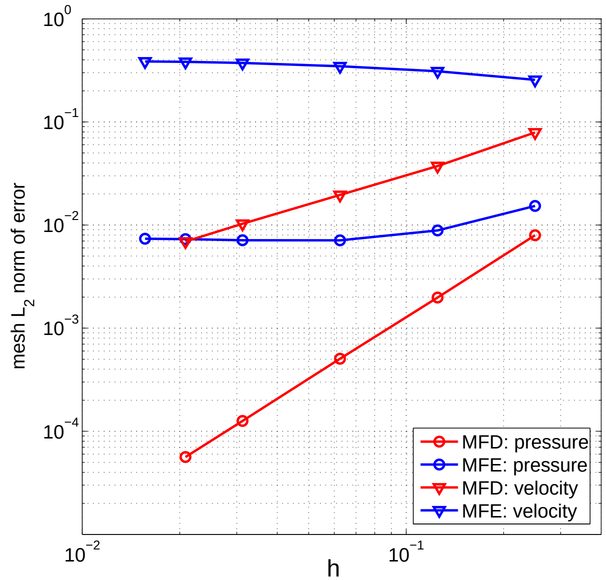
  where p^1 is a linear function and

$$[F^h,\, G^h]_E = \sum_{i,j=1}^{\#faces} \mathbb{M}_{E,ij}\, F^h_{f_i}\, G^h_{f_j}$$

- The matrix $\mathbb{M}_E$ is easily computed from geometric parameters of E and is not **unique**.

MFD method: generalized polyhedral meshes





- The mixed FE method does *not* converge on randomly perturbed meshes.
- The new MFD method has the optimal convergence rate.

MFD method: theoretical results

Our theoretical results include:

1. **For generalized polyhedral meshes we proved the optimal error estimates in mesh dependent L_2-norms:**

$$|||\boldsymbol{p}^{exact} - \boldsymbol{p}^{h}||| \leq C\, h^{2}, \qquad |||\boldsymbol{u}^{exact} - \boldsymbol{u}^{h}||| \leq C\, h.$$

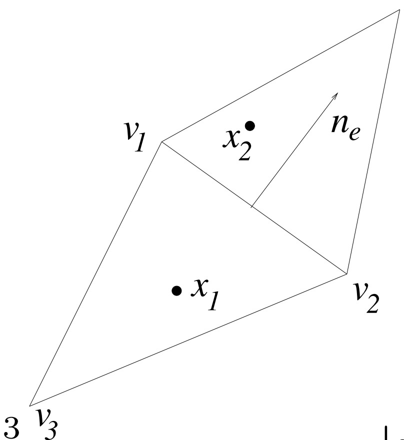
2. **We developed *a posteriori* error estimates for generalized polyhedral meshes.**

3. **We found and described a rich family of the MFD methods (e.g., a 6-parameter family for hexahedral meshes).**

4. **For simplicial meshes, we proved convergence of an explicit flux version of the MFD method. It results in a cell-centered discretization.**

Monotone finite volume method

$$\sum_{e \in \partial T} \boldsymbol{u}_e^h \cdot \boldsymbol{n}_e = \int_T Q \, \mathrm{d}x, \qquad \boldsymbol{u}_e^h = \frac{1}{|e|} \int_e \boldsymbol{u} \, \mathrm{d}s.$$



$$\boldsymbol{x}_1 = \sum_{i=1}^{3} \boldsymbol{v}_i \lambda_i, \quad \lambda_i = \frac{|\boldsymbol{n}_{\alpha(i)}|_{\mathbb{D}}}{\sum_{j=1}^{3} |\boldsymbol{n}_{\alpha(j)}|_{\mathbb{D}}}$$

Nonlinear two-point flux formula:

$$\boldsymbol{u}_e^h \cdot \boldsymbol{n}_e = A(p_{v_1}^h, p_{v_2}^h)\, p_{x_1}^h - B(p_{v_1}^h, p_{v_2}^h)\, p_{x_2}^h$$

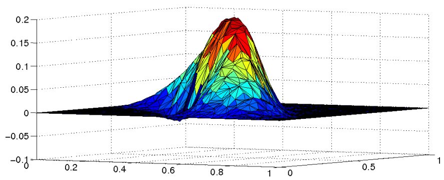
To compute $p_{v_1}^h$ and $p_{v_2}^h$, we use either

- ***linear interpolation* or**
- ***inverse weighting interpolation*,**

$$p_{v_1}^h = \sum_{T \ni \boldsymbol{v}_1} p_{x_T}^h w_T, \quad w_T = \frac{|\boldsymbol{x}_T - \boldsymbol{v}_1|^{-1}}{\sum_{T' \ni \boldsymbol{v}_1} |\boldsymbol{x}_{T'} - \boldsymbol{v}_1|^{-1}}.$$

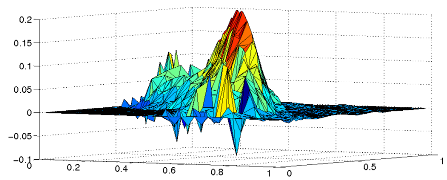
Monotone FV method: comparison

MFE method



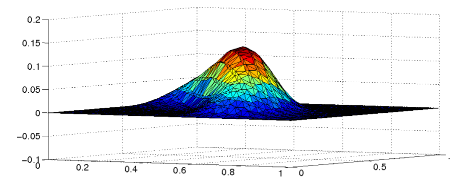
$p^h_{min} = -0.02$

MPFA method

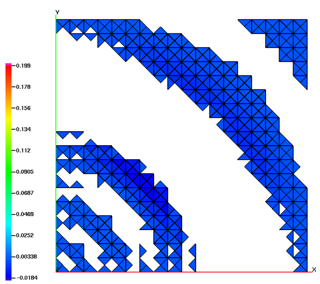


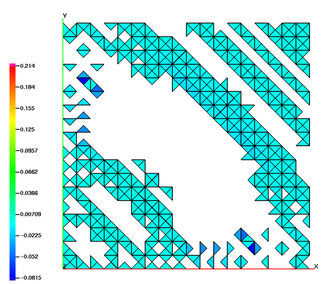
$p^h_{min} = -0.08$

nonlinear FV method



$p^h_{min} = 0$





$$Q(x,y) = \begin{cases} 1 & \frac{3}{8} \le x, y \le \frac{5}{8}, \\ 0 & \text{otherwise.} \end{cases}$$

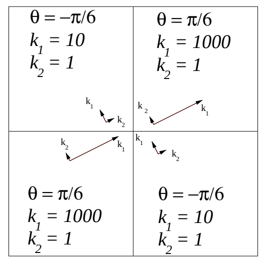
Location of negative values of p^h

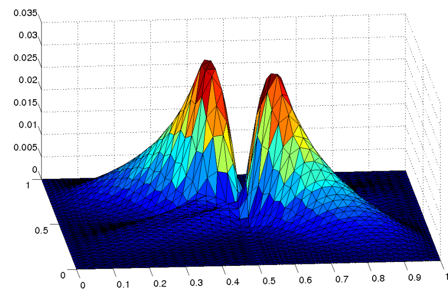
- **The diffusion tensor is anisotropic (ratio of eigenvalues is 200:1) and varies smoothly in space. The maximum principle implies that the continuum solution is positive.**

Monotone FV method: results

1. We proved monotonicity of the nonlinear FV method for stationary diffusion problems.

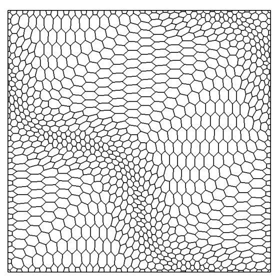
2. We improved stability of the method for problems with sharp gradients.

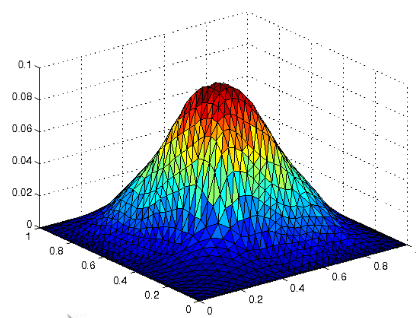




3. We developed a new *monotone* non-linear FV method for shape-regular polygonal meshes and isotropic diffusion tensors.

$$k_1/k_2 = 10$$





Discrete Maximum Principle

Constrained Quadratic Optimization Approach

$$\mathbf{div}\, A\, \mathbf{grad} u = 0 \ \text{ in } \Omega\,, \quad u = \gamma, \ \text{ in } \partial\Omega \rightarrow \max_{\partial\Omega} \gamma \leq u \leq \min_{\partial\Omega} \gamma$$

Dirichlet functional

$$D(u) = \int_\Omega (A \cdot \mathbf{grad} u, \mathbf{grad} u) dV \,, \quad \min_u D(u)$$

Triangular mesh, nodal discretization (piece-wise linear finite elements)
Discrete gradient

$$GRAD_T^x(U) = \frac{(U_1+U_2)(y_2-y_1)+(U_2+U_3)(y_3-y_2)+(U_3+U_1)(y_1-y_3)}{2V_T}$$

$$GRAD_T^y(U) = -\frac{(U_1+U_2)(x_2-x_1)+(U_2+U_3)(x_3-x_2)+(U_3+U_1)(x_1-x_3)}{2V_T}$$

Discrete Dirichlet functional

$$D[U] = \sum_T \left[\left(a_{xx} GRAD_T^x(U) + a_{xy} GRAD_T^y(U) \right) GRAD_T^x(U) + \left(a_{yx} GRAD_T^x(U) + a_{yy} GRAD_T^y(U) \right) GRAD_T^y(U) \right] V_T,$$

Constrained Quadratic Optimization

$$\min_{U_p} D[u]\,, \max_{\partial\Omega} \gamma \leq U_p \leq \min_{\partial\Omega} \gamma$$

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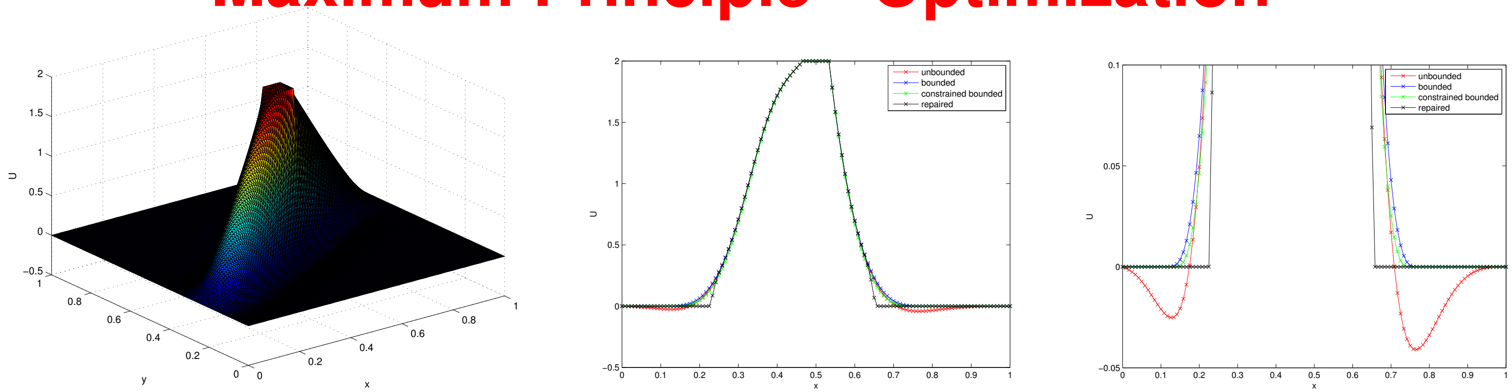
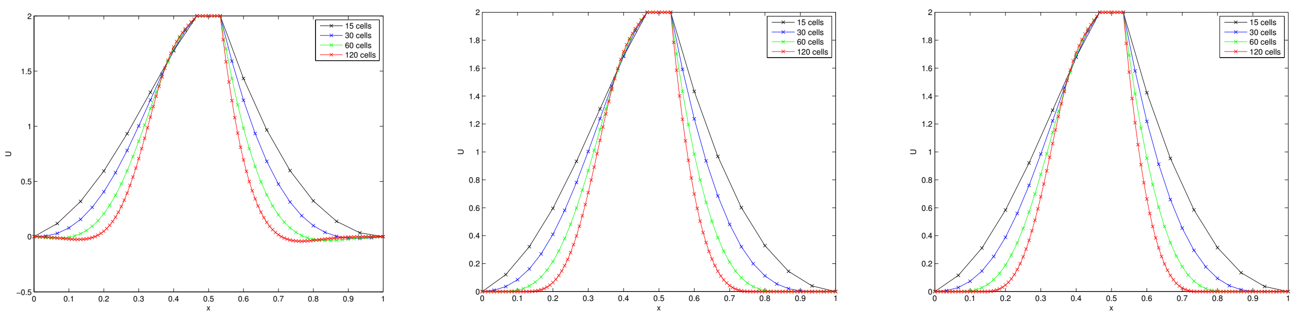
Maximum Principle - Optimization



Comparison of different methods



unbounded **bounded** **conser. unbounded**

Convergence study

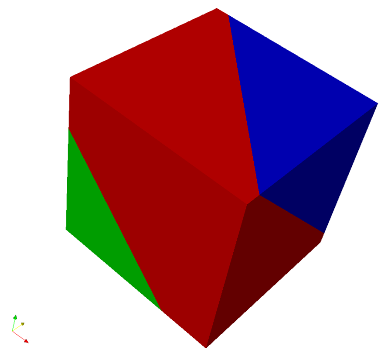
Closure Models for Multimaterial Arbitrary Lagrangian-Eulerian Methods (ALE)

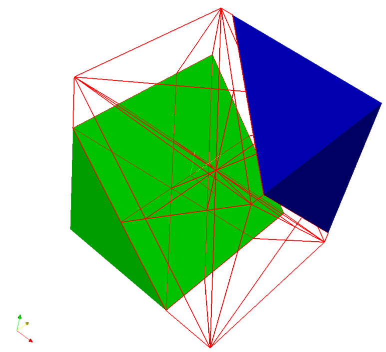
- **Lagrangian stage — Solving Lagrangian equations**
- **Rezone stage — Changing the mesh**
- **Remap stage — Conservative interpolation from Lagrangian to rezoned mesh**

- **Material interfaces may not coincide with mesh faces**
- **Mixed cells - cells which contain more than one material**

Multimaterial Lagrangian Hydro - Closure Models

- Single velocity for all materials - one velocity per node
- Each material has its own mass (density) and may have its own internal energy and pressure
- Each cell (including mixed cells) has to produce force to its vertices - one pressure to be used in momentum equation
- Closure model - how to produce this pressure and advance in time internal energy and density for each material





Mixed Zone Models - Classes of Models

Two Classes of Models

- Pressure Equilibrium — Pressure Relaxation (Explicitly enforced)
- Modeling Sub-Cell Dynamics

Mixed Zone Models - Design Principles

- If all materials in mixed cell initially have the same pressure — it is supposed to stay this way — preservation of contact
- Pressure Equilibrium — Pressure Relaxation (after some transition time pressures in mixed cells have to equilibrate)
- Conservation of Total Energy

Mixed Zone Pressure Equilibrium (Relaxation) Models

Pressure relaxation model :

$p_i^{n+\frac{1}{2}} + R_i^{n+\frac{1}{2}} = p^{n+\frac{1}{2}}$, $R_i^{n+\frac{1}{2}}$ **relaxation term**, $i-$**material index** , $n-$**time index**

Tipton's model (R. Tipton (LLNL) - unpublished notes, 1989)

Assumption — Isentropic

$$dS_i/dt = 0 \rightarrow d\mathcal{P}_i/dt = (\partial \mathcal{P}_i/\partial \rho_i)_{S_i}\, d\rho_i/dt = -\rho_i\, c_i^2\, (dV_i/dt)/V_i$$

$$p_i^{n+\frac{1}{2}} = p_i^n + (\delta t/2)\, d\mathcal{P}_i/dt \quad \rightarrow p_i^{n+\frac{1}{2}} = p_i^n - \rho_i^n\, (c_i^n)^2\, \delta V_i^{n+\frac{1}{2}}/V_i^n$$

Relaxation Term Resembles Viscosity

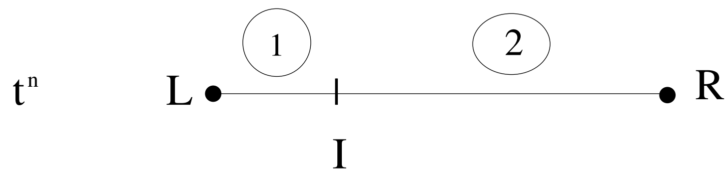
$$R_i = -l_i\, \rho_i\, c_i\, (\mathbf{divu})_i\ , \quad (\mathbf{divu})_i = (1/V_i)\,(dV_i/dt)$$

$$R_i^{n+\frac{1}{2}} = -\rho_i^n\, c_i^n (L^n/\delta t)\,(1/V_i^n)\, \delta V_i^{n+1}\, , L^n\ -$$ **characteristic length**

Closure Model

$$p_i^n - \rho_i^n\, (c_i^n)^2\, [1 + L^n/(c_i^n\, \delta t)]\, \delta V_i^{n+\frac{1}{2}}/V_i^n = p^{n+\frac{1}{2}}\, , \quad \sum_i \delta V_i^{n+\frac{1}{2}} = \delta V^{n+\frac{1}{2}}$$

Sub-cell Dynamics Approach to Closure Models



- **Each material can have it is own pressure**
- **There is no independent velocity of the interface — how to estimate it?** u_I **— interface velocity — acoustic Riemann solver**

$$u_I = [(\rho_1\, c_1)\, u_1 \; + (\rho_2\, c_2)\, u_2 \; + (p_1 - p_2)]/(\rho_1\, c_1 + \rho_2\, c_2)$$

Different choices for $u_1,\ u_2$ **are possible**

- **How to compute one pressure to be used in momentum equation?**
- **How to conserve total energy?**

Each material has its own "$p\, dV$**" equation**

$$m_i\, d\varepsilon_i/dt = -p_i\, dV_i/dt$$

Conservation of total energy argument is used to derive one pressure in mixed cell:

$$\frac{d}{dt}\left(\sum m_i\, \varepsilon_i\right) = m\,\frac{d\varepsilon}{dt} = -\sum p_i\,\frac{dV_i}{dt} = -p\,\frac{dV}{dt} \rightarrow p = \sum p_i\,\frac{dV_i}{dV}$$

Sub-cell Dynamics Approach to Closure Models

Questions:

- **How to define dV_i/dV ?**
- **What to do if $dV = 0$?**
- **What to do if some of dV_i/dV have different signs?**
  In this case averaged pressure can be negative even if all p_i are positive — not an average.

Design Principles

Find $\beta_i \sim dV_i/dV$, such that $1 \geq \beta_i \geq 0$ and $\sum \beta_i = 1$

Having β_i, we define $dV_i = \beta_i \, dV$, and therefore

$$\sum \frac{dV_i}{dt} = \frac{dV}{dt} \cdot \sum \beta_i = \frac{dV}{dt}\,, \qquad p = \sum \beta_i \, p_i$$

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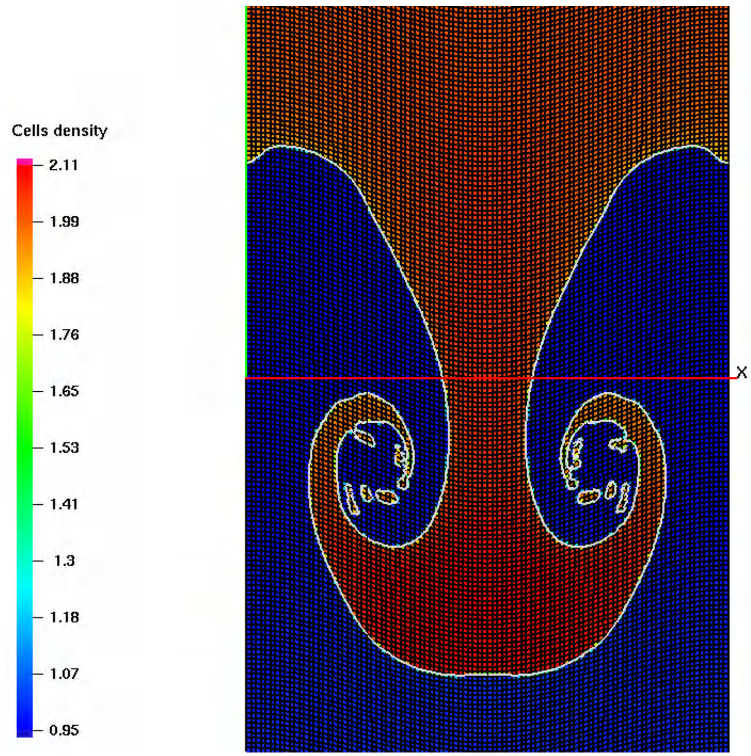
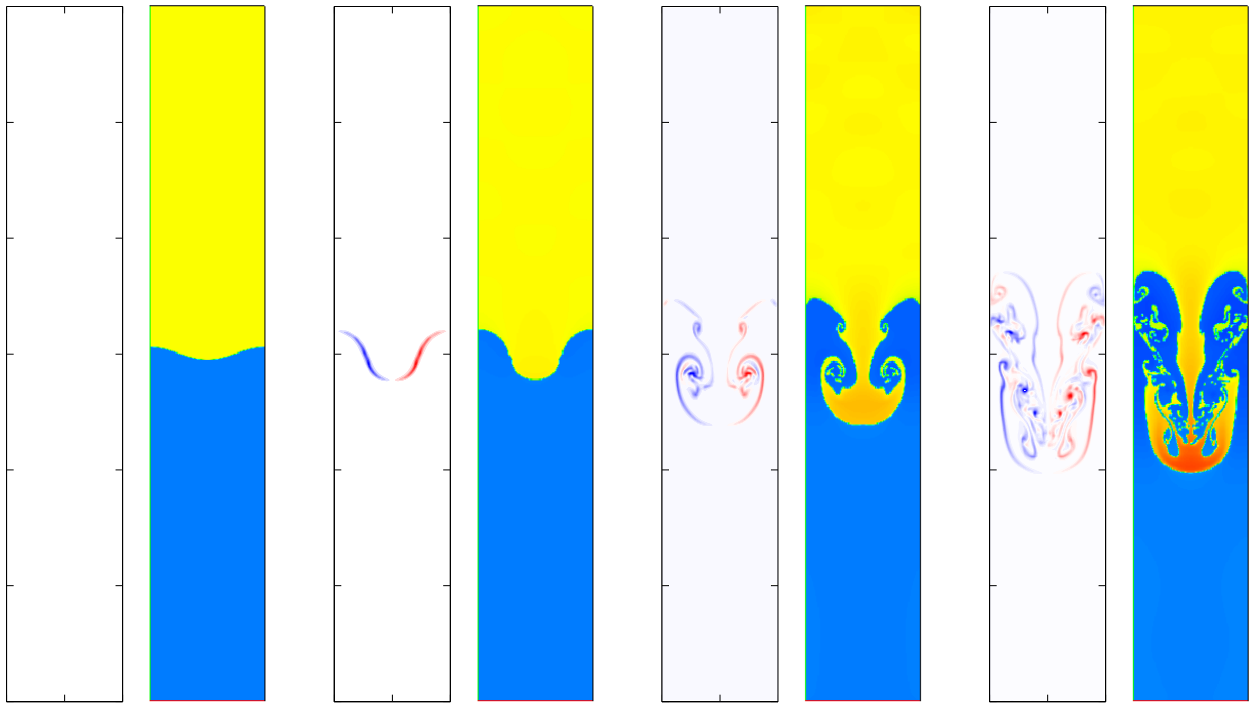
Example of Rayleigh-Taylor Calculation
LANL ASC Code-FLAG



Eulerian=Lagrange+Remap; Interface Reconstruction — Mixed cells

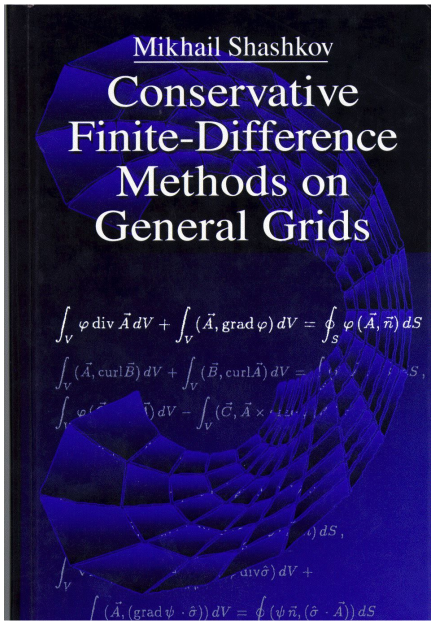
Example of Rayleigh-Taylor Calculation

LANL ASC Code-FLAG



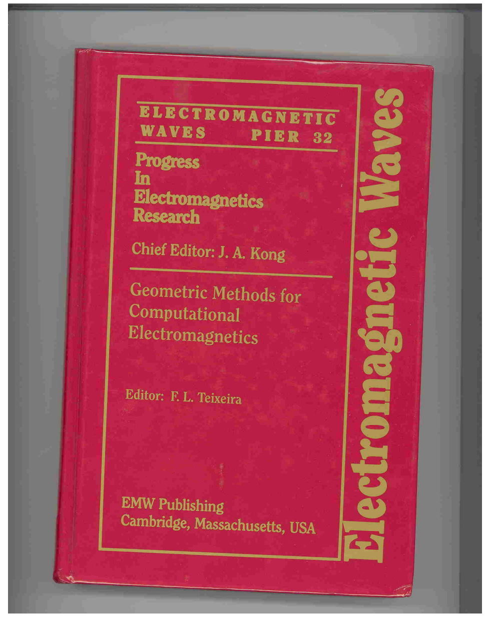
Vorticity and Density

Outreach

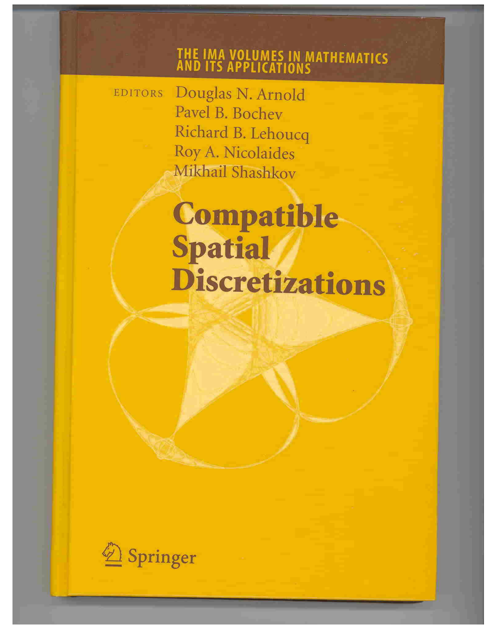


M. Shashkov

Book on Support-Operators Method



Chapter 4. Mimetic Finite Difference Methods for Maxwell's Equations and Equations of Magnetic Diffusion
(J. Hyman and M. Shashkov)



IMA Workshop: Compatible Spatial Discretizations for PDEs Supported by DOE and NSF

D. Arnold, P. Bochev, R. Lehoucq, R. Nicolaides, M. Shashkov

Organizers and Co-editors of special IMA Volume

Outreach

- Publications: 7 (2002), 5 (2003), 14 (2004), 9 (2005), 10 (2006)
- Workshop on Mimetic Discretizations of Continuum Mechanics, 2003, San Diego State University
- IMA "Hot Topics" Workshop — Compatible Spatial Discretizations for PDEs May 11-15, 2004, Institute for Mathematics and its Applications, University of Minnesota
- Second Venezuelian Workshop on Mimetic Discretizations, 2004
- LACSI (Los Alamos Computer Science Institute) Symposium 2004 — Mimetic Methods for PDEs and Applications, Santa Fe, NM
- A CMA (Centre of Mathematics and Applications) Workshop on Compatible Discretizations for PDEs — University of Oslo

How do we train the future workforce?

- **Create successful research teams - Numerical Analysis Team (T-7, LANL)**
- **Collaborative work between academia and Labs - UT Austin, UC Davis, Pavia, UNM, SDSU, Prague Tech. Univ., Munich Tech. Univ., U. Pittsburg, SNL,LLNL, AWE, CEA, U. Bordeaux, U. Toulouse, Texas A & M, U. Houston, Institute of Numerical Mathematics, Moscow.**
- **Promoting Lab internship for undergrads and grads: The Los Alamos Mathematical Modeling and Analysis Student Program (Mostly funded by ASC)** * To offer strong scientific guidance and close mentor-student relationships while providing the students with training and experience in interdisciplinary research in the mathematical sciences. * To bridge the gap between fundamental research and applied technology and create a program for introducing young scientists, in the formative stages of their careers, to important problems derived from research in interdisciplinary applied mathematics. * To provide a strong link for effective collaboration of Los Alamos scientists with academic centers of excellence in the mathematical sciences.
- **UTEP Winter (January 2008) School on Computational Science for graduate and Ph.D. students from US and abroad (P. Solin — main organizer). In particular P. Bochev and I will give lectures on compatible and mimetic discretizations.**

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Conclusion

- We have created solid mathematical foundation of the Mimetic Finite Difference Methods
- Mimetic Finite Difference Methods
  as Powerful as Finite Volume Methods and Finite Element Methods
- Applications of the Mimetic Finite Difference Methods
  - Fluid and solid mechanics
  - Shock physics
  - Electromagnetism
  - Radiation Transport
  - General Relativity
  - Flow in Porous Media
  - Laser Plasma Simulations
  - Computational Geometry
  - Image Analysis
  - Astrophysics
- Information ?
  shashkov@lanl.gov; webpage: cnls.lanl.gov/$\sim$ shashkov