

LA-UR-09-04359

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<i>Title:</i>	Accurate Direct Eulerian Simulation of Dynamic Elastic-Plastic Flow
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<i>Intended for:</i>	Joint U.S.-Russia Conference on Advances in Materials Science 30 August – 04 September 2009 Prague, Czech Republic



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# Accurate Direct Eulerian Simulation of Dynamic Elastic-Plastic Flow

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Joint US-Russia Conference on Advances in Materials Science  
Prague, Czech Republic  
31 August – 3 September 2009

# Outline of this presentation

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- A new and accurate approach for large-strain Eulerian thermoelasticity.
- The standard *hypoelastic* Eulerian approach: there are fundamental problems with these equations.
- The *hyperelastic* Eulerian approach: as of today, we know of no algorithms that *accurately* solve this fully conservative set of equations.
- The Flux Distribution method: developed for MHD, this approach is ideal for Eulerian hyperelasticity.
- Summary

*This presentation uses only words and equations to describe this new approach, but contains no computational results.*

# We propose a new approach for accurate direct Eulerian simulation of dynamic elastic-plastic flow.

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- Why is this important?
  - The standard (hypoelastic) approach for Eulerian thermoelasticity has fundamental problems.
  - For example, conservation is not maintained — this is particularly important for shock waves.
- What is the new approach?
  - This approach incorporates the recent “Flux Distribution” method.
  - This method was developed for — and successfully demonstrated on — Eulerian MHD, which has the constraint:  $\operatorname{div} \mathbf{B} = 0$ .
  - The same ideas can be applied to large-strain Eulerian thermoelasticity, which has the similar constraint:  $\operatorname{curl} \mathbf{g} = \mathbf{0}$ .
- Has anyone already tried or implemented this approach?
  - No! But this research could directly affect many simulations.

# What are the standard equations of motion for dynamic solid response?

- The standard conservation laws for thermoelasticity\* are used in (almost all) Eulerian schemes.
  - This is a quasi-linear system in terms of the Cauchy stress:

$$\text{Mass:} \quad \dot{\rho} + \rho v^j_{;j} = 0 \quad \rho = \text{mass density}$$

$$\text{Momentum:} \quad \rho \dot{v}^i - \sigma^{ij}_{;j} = 0 \quad v^i = \text{velocity} \quad \sigma^{ij} = \text{Cauchy stress}$$

$$\text{(Internal) Energy:} \quad \rho \dot{\varepsilon} - \sigma^{ij} d_{ij} = 0 \quad \varepsilon = \text{specific internal energy}$$

- Typically, these equations are augmented by *hypoelastic constitutive laws* (incremental Hooke's law):

$$\text{Stress evolution equations} \begin{cases} -\dot{p} = K \operatorname{tr} \mathbf{d} \\ \dot{s}_{ij} = 2G \operatorname{dev}(\mathbf{d})_{ij} \end{cases} \quad \text{where} \quad \begin{cases} \mathbf{d} \equiv \operatorname{sym}(\nabla \mathbf{v}) = \text{rate of deformation} \\ \boldsymbol{\sigma} \equiv -p\mathbf{I} + \mathbf{s} \leftarrow \text{stress deviator} \end{cases}$$

- In 3D, these are 11 equations for 11 unknowns:

$$\rho, \varepsilon, v^i, \sigma^{ij}$$

\* Plohr, B.J., Plohr, J.N., "Large Deformation Constitutive Laws for Isotropic Thermoelastic materials," LANL Report LA-UR-05-5471 (2005).

## What are some problems with this approach?

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- For the hypoelastic model, the current stress: (1) is a functional of deformation history, and (2) its value depends strongly on the numerical method used.
- Thermodynamic consistency is often a problem.
  - The moduli  $K$  and  $G$  are often assumed constant: not consistent.
  - One should calculate  $K$ ,  $G$  (+ missing terms) as derivatives of the free energy with respect to the (non-linear) strain tensor.
- The momentum equation is not frame indifferent.
  - “Frame indifferent” means that a rigid-body motion does not change the results.
  - The standard way to address this problem is to replace the material time rate with an objective time rate.
  - But there are many different objective rates. Which objective rate should one use? What is the correct right hand side?
  - How does one consistently model nonlinear thermo-elastic effects?

## What else is wrong with the standard approach?

- These standard quasi-linear equations are not in conservation form (important for shock waves).
  - This leads to numerical inaccuracy and non-physical behavior.
  - Stress is not a conserved quantity (which one should evolve).
- Plohr & Plohr\* (P&P) document the errors in this approach.
  - P&P show that the full, correct equations can be written:

Vorticity tensor  $\rightarrow$

$$-\dot{p} = K \operatorname{tr} \mathbf{d} + b_{v,s}^{kl} \operatorname{dev}(\mathbf{d})_{kl} \quad (1)$$

$$\dot{s}^{ij} - \omega^i_k s^{kj} - s^{ik} \omega^j_k = b_{v,s}^{ij} \operatorname{tr} \mathbf{d} + b_{s,s}^{ijkl} \operatorname{dev}(\mathbf{d})_{kl} \quad (2)$$

- There are 4 main differences, *all of approx. the same magnitude*, between these equations and the usual hypoelastic formulation.
- One difference is accounted for: the Z-J objective rate (LHS of (2)).
- The other differences (i.e., RHS of (1,2)) are *not* accounted for.
- The RHS of (1,2) depends on the inverse deformation gradient  $\mathbf{g}$ , which is *not computed* in the standard approach.

$b^{ijkl}$  = Birch-Wallace elasticity tensor

\* Plohr, B.J., Plohr, J.N., "Large Deformation Constitutive Laws for Isotropic Thermoelastic materials," LANL Report LA-UR-05-5471 (2005).

# Nonlinear thermoelasticity can be described by a set of fully conservative equations.

- The 1st order system of (true) conservation laws is:

Mass:  $\rho_{;t} + (\rho v^j)_{;j} = 0$

Momentum:  $(\rho v^i)_{;t} + (\rho v^i v^j - \sigma^{ij})_{;j} = 0$

(Total) Energy:  $(\rho e)_{;t} + (\rho e v^j - v_i \sigma^{ij})_{;j} = 0$

Eulerian Continuity:  $(g^\alpha_i)_{;t} + (g^\alpha_i v^i)_{;j} = 0$

Stress evolution is replaced by  $g^\alpha_i$  evolution.

The specific total energy is:

$$e \equiv \frac{1}{2} v_k v^k + \varepsilon$$

The inverse deformation gradient is:

$$g^\alpha_i \equiv \frac{\partial X^\alpha}{\partial x^i}$$

Material (Lagrangian) index

This gradient must satisfy the constraint:  $\varepsilon_i{}^{jk} g^\alpha_{j;k} = 0$

Permutation symbol:  
 $\varepsilon_{ijk} = \varepsilon_i{}^{jk} = \dots$

- In 3D, this set of relations has 14 fundamental equations for the following 14 unknowns:

$$\varepsilon \Leftrightarrow \rho, \theta, v^i, g^\alpha_i$$

# There are two non-standard elements in this hyper-elastic formulation.

1. Thermoelastic model is based on the Helmholtz free energy  $\psi$ :

Free Energy:

$$\psi = \psi(\mathbf{E}, \theta)$$

Lagrangian strain tensor

Stress Tensor:

$$\sigma^{ij} \equiv \rho F^i_{\alpha} (\partial \psi / \partial E_{\alpha\beta})|_{\theta} F^j_{\beta}$$

Specific Entropy:

$$\eta \equiv -(\partial \psi / \partial \theta)|_E$$

Deformation gradient

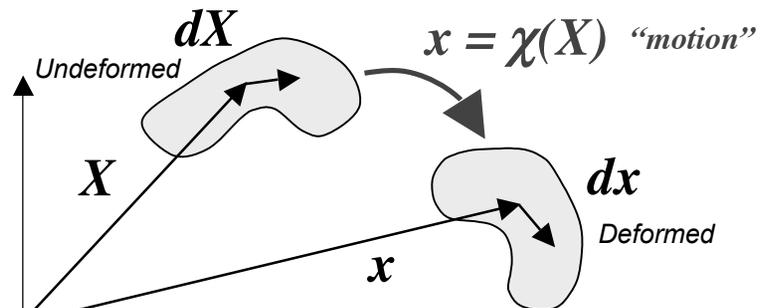
Specific Internal Energy:

$$\varepsilon = \psi + \eta \theta$$

- Consistency — thermodynamic, kinematic, and dynamic — is automatically enforced with this model in the conservation laws.

2. The inverse deformation gradient maps back to the undeformed configuration.

- The constraint comes from using both  $\mathbf{v}$  and  $\mathbf{g}$  as independent variables, which is required to write a 1st-order system of eq'ns.



$$g^{\alpha}_i \equiv \partial X^{\alpha} / \partial x^i = (F^i_{\alpha})^{-1}$$

## This fully conservative formulation can be extended to viscoplasticity.

- It is straightforward to add viscoplastic response.

- Add a plastic state vector  $U^P$  to the free energy:

$$\psi = \psi(\mathbf{E}, \theta, U^P) \quad U^P = U^P(\mathbf{E}^P, \kappa, \dots)$$

- Add conservation laws (advection + source) for  $U^P$  :

$$(\rho U^P)_{;t} + (\rho U^P v^j)_{;j} = \rho S^P$$

Plastic strain

Internal state variables

- Like the thermoelastic model, this viscoplastic modeling is deformation- or strain-based.
- Strain-based modeling is advantageous for highly nonlinear phenomena, such as such as elastic phase change or multiaxial (e.g., polycrystal) plasticity.

# The “Flux Distribution” approach leads to an algorithm that preserves a critical constraint.

- Eulerian continuity equations imply an intrinsic constraint: the curl of the elements of  $g$  are zero:  $\varepsilon_t^{jk} g_{j;k}^\alpha = 0$ . Permutation symbol
  - If a solution is curl-free at  $t = 0$ , then it is curl-free for  $t > 0$ .
  - This is formally similar to the  $\operatorname{div} \mathbf{B} = 0$  constraint in MHD. “Intrinsic constraint”
  - How can one include this important property in a cell-centered, Godunov scheme?
- Flux Distribution approach: M. Torrilhon\* (ETH-Zürich).
  - Main idea: calculate the *distribution* of fluxes in the *complete neighborhood* of a given computational cell.
  - Combine all of these fluxes so that the intrinsic constraint is enforced *discretely*.
  - More precisely, the constraint is enforced exactly and locally.
  - This approach is independent of *how* the fluxes are computed.
    - For example, you can use any Riemann solver that you choose.

# The Flux Distribution basis depends on the particular constraint equation.

- A finite volume scheme can be written:

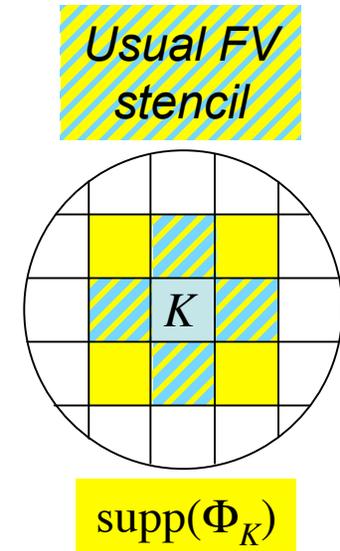
$n$  is a time index

$K$  is a spatial index, e.g., in 2D,  $K = (i,j)$

$$U^{n+1}|_K = U^n|_K + \sum_{L \in \text{supp}(\Phi_K)} \Phi_L(U^n)|_K$$

The flux between cell  $K$  and all of its neighbors

Sum over the complete neighborhood of cell  $U_K$



- One decomposes the Flux Distribution as:

Shape functions  $\underline{\Phi}$  are independent of  $U$

Scalar coefficients  $\varphi$  are dependent on  $U$

$$\Phi_L(U) = \sum_{\ell} \varphi_L^{(\ell)}(U) \underline{\Phi}_L^{(\ell)}$$

- One must derive a discrete approximation  $\underline{C}$ , corresponding to the continuous constraint equation  $C(U) = \mathbf{0}$ , that satisfies:

$$\underline{C}_K \cdot \underline{\Phi}_L^{(\ell)} = 0, \quad \forall L \in \text{supp}(\Phi_K), \quad \forall \ell, \quad \text{i.e.,} \quad \underline{\Phi}_L^{(\ell)} \in \ker(\underline{C}_K)$$

- For the elasticity case, this constraint is  $\text{curl } g = \mathbf{0}$  — but we have not worked out the details yet, nor has anyone else...

## The Flux Distribution concept has been developed for other sets of equations.

- The construction of an algorithm reduces to: (1) designing a mimetic discrete constraint operator, and (2) embedding this operator in a stable conservative difference scheme.
- Example\*: the system of 2D non-linear wave equations:

$$\left. \begin{array}{l} \rho_{;t} + \operatorname{div} \mathbf{u} = 0 \\ \mathbf{u}_{;t} + \operatorname{grad} p(\rho) = \mathbf{0} \end{array} \right\} + \text{constraint: } C(\mathbf{u}) = \operatorname{curl} \mathbf{u} = \mathbf{0}$$

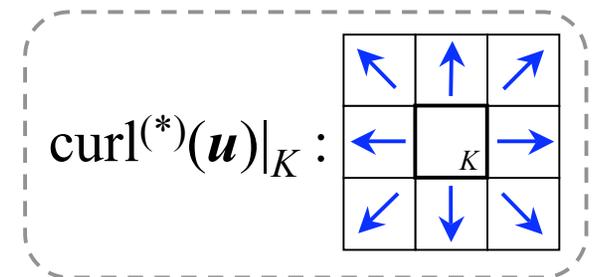
- The continuous curl operator  $C$  is discretized to  $\underline{C} = \operatorname{curl}^{(*)}$  as:

$$\operatorname{curl}^{(*)}(\mathbf{u})|_{i,j} = (1/2) (\{\zeta_{i+1,j}\}_y - \{\zeta_{i-1,j}\}_y)/\Delta x + (1/2) (\{\zeta_{i,j+1}\}_x - \{\zeta_{i,j-1}\}_x)/\Delta y$$

where the  $y$ -direction averaging operator  $\{\cdot\}_y$  is defined as:

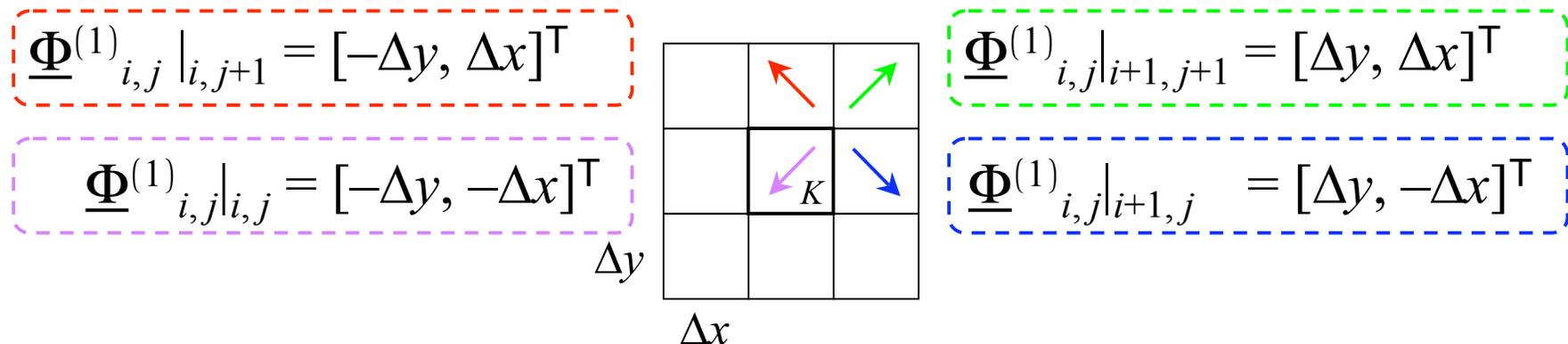
$$\{\zeta_{i,j}\}_y \equiv (1/4) (\zeta_{i,j+1} + 2\zeta_{i,j} + \zeta_{i,j-1})$$

and similarly for the  $x$ -direction operator  $\{\cdot\}_x$



## The shape functions are determined by the null space of the discrete constraint operator.

- Recall that the shape functions (i) determine the differencing scheme and (ii) obey the constraint intrinsically.
- Here, the nullspace of  $\text{curl}^{(*)}(\mathbf{u})|_{i,j}$  is four-dimensional.
- One element,  $\underline{\Phi}^{(1)}_{i,j}$ , vanishes *except* in the upper right quadrant of the  $3 \times 3$  stencil that is centered at cell  $K=(i,j)$ :



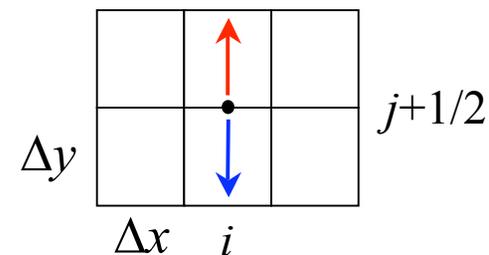
- The other elements,  $\underline{\Phi}^{(2)}_{i,j}$ ,  $\underline{\Phi}^{(3)}_{i,j}$ ,  $\underline{\Phi}^{(4)}_{i,j}$ , are similar, but they are centered on the other corners of cell  $K$ .

## For this case, we can compare the classical and curl-preserving finite volume schemes.

- The classical  $y$ -momentum update is written in terms of edge FDs as:

$$\underline{\Phi}^{(\text{class})}_{i,j+1/2} |_{i,j} = (\Delta t / \Delta y) p_{i,j+1/2} [0, -1]^T$$

$$\underline{\Phi}^{(\text{class})}_{i,j+1/2} |_{i,j+1} = (\Delta t / \Delta y) p_{i,j+1/2} [0, 1]^T$$



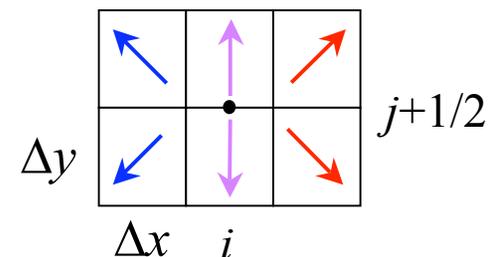
$$U^{n+1} \Big|_K = U^n \Big|_K + \sum_{L \in \text{supp}(\Phi_K)} \Phi_L(U^n) \Big|_K$$

- There are similar expressions at the other edges

- Instead, the curl-preserving FD at this edge is given by:

$$\underline{\Phi}^{(\text{curl-free})}_{i,j+1/2} |_{i,j} = (\Delta t / (\Delta x \Delta y)) p_{i,j+1/2} ( \underline{\Phi}^{(1)}_{i,j} |_{i,j} + \underline{\Phi}^{(2)}_{i,j} |_{i,j} ) / 8$$

- The classical  $y$ -momentum update is not curl-preserving, since it can not be written as a linear combination of  $\{ \underline{\Phi}_K^{(\ell)} \}$ .



# There are three main theoretical elements of this approach. (1/2)

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1. The strain-based material modeling framework.
  - This part is well developed: there are many papers that describe strain-based elasto-plasticity.
  - Existing stress-based models can be put in this form.
  - R. Menikoff (LA-UR-03-0047-rev, LA-UR-1505-rev) gives a detailed development of the conservative framework and elastic-plastic wave analysis.
  - B. Plohr & J. Plohr (LA-UR-05-5471, LA-UR-05-6333) give a detailed discussion of an isotropic, thermoelastic model for 3<sup>rd</sup>-order energy with volumetric / deviatoric decomposition.
2. The Flux Distribution method:
  - This element is not well developed (yet) for thermoelasticity.
  - In other words, this will require additional development.
  - M. Torrilhon developed this method extensively in 2D for MHD and other systems — but *not* thermoelasticity / viscoplasticity.

# There are three main theoretical elements of this approach. (2/2)

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## 2. The Flux Distributions method (continued)

- Elastoplasticity: appropriate operators and numerical schemes have not yet been developed.
  - 2D: should be fairly straightforward.
  - 3D: the three vector curl-constraints are a completely new issue.

## 3. Various computational aspects

- These aspects are both complicated and intricate.
- A conservative elasto-plastic framework was implemented by G. Miller & P. Colella: *J. Comput. Phys.* **167**:131–176 (2002).
  - This scheme is **not** constraint-enforcing; rather, the magnitude of constraint error is reduced by diffusing it artificially.
  - The flux distribution method should be superior to this approach.
- We have begun implementing the basic cell-centered Godunov machinery in a research code.
  - This code already has hyper-elastic constitutive models.

## Summary of this presentation

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- We described a new and accurate approach for large-strain Eulerian thermoelasticity / viscoplasticity.
- There are fundamental problems with the standard hypoelastic Eulerian approach.
- The hyperelastic Eulerian approach: no algorithms accurately solve this fully conservative set of equations.
- The Flux Distribution approach: this approach (developed for MHD) is perfect for Eulerian hyperelasticity.
- We have outlined this new and accurate approach, but much work remains to be done:
  - We must develop the appropriate operators that discretely enforce the  $\text{curl } \mathbf{g} = \mathbf{0}$  constraint.
  - We must embed those operators in a conservative elasto-plastic algorithmic framework.

# Abstract

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The simulation of dynamic, large strain, multi-material deformation and failure is an important, difficult, and unsolved computational challenge. Material models for solids are most easily represented in the Lagrangian (material-fixed) frame. Many problems cannot be simulated with a conventional Lagrangian approach because the mesh cannot accommodate large shear strain and material rotation. Simulation in the Eulerian (space-fixed) frame is not subject to Lagrangian mesh distortion issues. However, existing Eulerian schemes suffer from unsolved difficulties when solid materials are involved. One fundamental issue is that Eulerian schemes typically treat only the fluid variables (mass density, momentum, and fluid energy) in conservation form. Such formulations do not represent all of the conservation laws that govern the material motion.

We propose a different scheme in which the entire system of large-strain, elasto-visco-plasticity equations in the Eulerian frame is written in first-order conservation form. This system contains an intrinsic constraint that must be discretely enforced. Standard Godunov-type schemes cannot satisfy this constraint. A recently developed approach, the method of Flux Distributions, has been devised to discretely enforce this type of constraint for numerical schemes with cell-centered variables. Numerical results for magnetohydrodynamics (MHD) simulations have demonstrated that this approach exactly enforces the divergence-free constraint on the magnetic field.

We present a non-linear, hyperelastic constitutive framework that allows for large elastic volumetric strain together with modern, large-strain, thermo-visco-plastic models. For these equations, the necessary constraint is that the curl of the inverse deformation gradient vanishes identically. This constraint arises from the necessary compatibility conditions between the velocity and the deformation gradient. To our knowledge, no other algorithm for elasto-visco-plasticity accurately enforces this constraint.

This presentation describes the foundations of this approach, including a motivation of the underlying equations. We explain how to develop a Flux Distribution algorithm for these equations. As this approach is new and novel, we do not yet have any numerical results to validate our claims. This presentation comprises the first installment in our program to develop this new method for computational solid dynamics.