An explicit pseudo-energy conservative scheme for contact elastodynamics

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Context

- **Motivations**:
  - Effects of an explosion on a structure: coupling between a mobile, deformable structure and compressible fluid flow (Finite Volumes)
    - ⇒ *Rigid, deformable, possibly fracturing structure, with self-contact*
      - Solid time-step cannot be chosen independently from the fluid
  - Effect of overpressure and fragments
- **Main ideas**:
  - Explicit in time coupling scheme, conserve fluid mass, energy, momentum
  - Focus here: Consistent solid particle method with energy and momentum preservation
- **Long-term collaboration with CEA**:
  - Lagrangian code Mka3d for elasticity (C. Mariotti 2006-), 2d fluid-structure coupling (PhD LM 2008-2011), PhD A. Puscas on 3d deformable coupling with fracturation (2011-2014), PhD F. Marazzato on plasticity and dynamic fracturation (2016-2020)
  - ANR JCJC grant: PhD N. Dirani on coupling with contact (2018-2022), post-doc S. McGovern on local time-stepping and parallelization (2020-2021)
  - Current development of 3d code at Inria (AMDT)

Outline

Plan

Energy preserving schemes: brief state of the art

- Geometric numerical integration (Hairer Lubich Wanner 06)
  - e.g. symplectic schemes
  - Conservation of an approximate energy over long times
  - Different from energy conservation (e.g. Zhong Marsden 88)
  - Usually requires constant time-steps
- Energy-momentum conserving schemes (Simo *et al.*, *CMAME* 92)
  - Exact conservation of energy and momentum
  - Implicit schemes, find an appropriate quadrature point in time
  - Nonlinear system, Newton-Raphson iterations
- Present result: first example of an explicit pseudo-energy conserving scheme for split Hamiltonian systems (Marazzato Ern Mariotti LM, *CMAME* 19)
- Recent alternative explicit energy conserving scheme (Bilbao Ducceschi Zama, *JCP: X* 23)

MEMM scheme

- Hamiltonian in split form (q=position, $p = Mv$=momentum, M symm. def. pos.):

$$H(q, p) = \frac{1}{2} p^T M^{-1} p + V(q)$$

- Hamiltonian dynamics:

$$\dot{q} = M^{-1} p, \quad \dot{p} = -\nabla_q V(q) =: F(q)$$

- MEMM scheme:

$$q^{n+1} = q^n + \Delta t M^{-1} p^{n+1/2}$$

$$p^{n+3/2} = p^{n-1/2} + 2\Delta t \int_0^1 F(q^n + \tau \Delta t M^{-1} p^{n+1/2}) \mathrm{d}\tau.$$

- Main idea: Inertial mouvement of particle during the time-step, exact time-integration of the generated force $q^{n+\tau} = q^n + \tau \Delta t M^{-1} p^{n+1/2}$
- Exact conservation of the following pseudo-energy:

$$\tilde{H}^n = \frac{1}{2} (p^{n-1/2})^T M^{-1} p^{n+1/2} + V(q^n).$$

Proof of conservation (MEMM scheme)

- Conservation of momentum $Q^n = c^T p^n$:
    - c a constant vector such that $\forall h \in \mathbb{R},\ V(q + hc) = V(q)$, $p^n = (p^{n+1/2} + p^{n-1/2})/2$:

$$Q^{n+1} - Q^n = \frac{1}{2} c^T (p^{n+3/2} - p^{n-1/2}) = -\Delta t \int_0^1 c^T \nabla_q V(q^{n+\tau}) \mathrm{d}\tau$$

$$= -\int_0^{\Delta t} \frac{1}{h} \left(V(q^{n+\tau} + hc) - V(q^{n+\tau}) + o(h) \right) \mathrm{d}\tau = 0.$$

- Conservation of pseudo-energy $\tilde{H}^n = \frac{1}{2}(p^{n-1/2})^T M^{-1} p^{n+1/2} + V(q^n)$:
    - Note that $V(q^{n+1}) - V(q^n) = \Delta t \int_0^1 (M^{-1} p^{n+1/2})^T \nabla_q V(q^{n+\tau}) \mathrm{d}\tau$:

$$\tilde{H}^{n+1} - \tilde{H}^n = \frac{1}{2}(M^{-1} p^{n+1/2})^T (p^{n+3/2} - p^{n-1/2}) + V(q^{n+1}) - V(q^n)$$

$$= -\Delta t (M^{-1} p^{n+1/2})^T \int_0^1 \nabla_q V(q^{n+\tau}) \mathrm{d}\tau$$

$$+ \Delta t \int_0^1 (M^{-1} p^{n+1/2})^T \nabla_q V(q^{n+\tau}) \mathrm{d}\tau = 0$$

Control on the pseudo-energy

- Exact energy $H^n = \frac{1}{2}(p^n)^T M^{-1} p^n + V(q^n)$ with

$$p^n = (p^{n+1/2} + p^{n-1/2})/2.$$

- Difference between the exact energy and the pseudo-energy:

$$H^n - \tilde{H}^n = \frac{1}{8}\left(p^{n+1/2} - p^{n-1/2}\right)^T M^{-1}(p^{n+1/2} - p^{n-1/2}) \geq 0.$$

- In addition,

$$p^{n+3/2} - p^{n+1/2} = -(p^{n+1/2} - p^{n-1/2}) + 2\Delta t \int_0^1 \nabla_q V(q^{n+\tau})d\tau,$$

so that

$$\|p^{n+3/2} - p^{n+1/2}\| \leq \|p^{n+1/2} - p^{n-1/2}\| + 2\Delta t\|\nabla_q V\|_{L^\infty},$$

and $H^n - \tilde{H}^n = O(\Delta t^2)$.

Bilbao *et al.* scheme

- Assumption: positive (lower bounded) potential energy V
- Set $V = \frac{1}{2}\psi^2$ and $g = \frac{1}{\sqrt{2V}}\nabla_q V$
- Linearly implicit scheme:

$$q^{n+1} = q^n + \Delta t M^{-1} p^{n+1/2}$$

$$p^{n+1/2} = p^{n-1/2} - \frac{\Delta t}{2} g^n(\psi^{n+1/2} + \psi^{n-1/2}), \quad g^n = \frac{1}{\sqrt{2V(q^n)}}\nabla_q V(q^n)$$

$$\psi^{n+1/2} = \psi^{n-1/2} + \frac{1}{2}(g^n)^T(q^{n+1} - q^{n-1}).$$

- Can be explicitly solved using Sherman-Morrison inversion formula

Proof of conservation (Bilbao *et al.* scheme)

- Conservation of momentum $Q^{n+1/2} = c^T p^{n+1/2}$:
  - c a constant vector such that $\forall h \in \mathbb{R}$, $V(q + hc) = V(q)$:

$$Q^{n+1/2} - Q^{n-1/2} = c^T(p^{n+1/2} - p^{n-1/2}) = -\frac{\Delta t}{2}(\psi^{n+1/2} + \psi^{n-1/2})c^T g^n$$

$$= -\frac{\Delta t}{2} \frac{\psi^{n+1/2} + \psi^{n-1/2}}{\sqrt{2V(q^n)}} c^T \nabla_q V(q^n)$$

$$= -\frac{\Delta t}{2} \frac{\psi^{n+1/2} + \psi^{n-1/2}}{\sqrt{2V(q^n)}} \frac{V(q^n + hc) - V(q^n) + o(h)}{h} = 0.$$

- Conservation of energy $H^{n+1/2} = \frac{1}{2}(p^{n+1/2})^T M^{-1} p^{n+1/2} + \frac{1}{2}(\psi^{n+1/2})^2$:
  - Using the fact that the energy is quadratic in p and ψ, and setting:

$$p^n = (p^{n+1/2} + p^{n-1/2})/2, \quad \psi^n = (\psi^{n+1/2} + \psi^{n-1/2})/2,$$

$$H^{n+1/2} - H^{n-1/2} = (p^n)^T M^{-1}(p^{n+1/2} - p^{n-1/2}) + \psi^n(\psi^{n+1/2} - \psi^{n-1/2})$$

$$= -\Delta t \psi^n (p^n)^T M^{-1} g^n + \psi^n (g^n)^T \frac{q^{n+1} - q^{n-1}}{2} = 0.$$

Comparison between the two schemes

MEMM scheme

- Exact integration on a path, needs quadrature (in practice, GL2 or GL3 work fine)
- Pseudo-energy: can be negative
- Conservation at integer steps
- Prioritize exact potential energy
- Control on position q through V
- Control on $H^n - \tilde{H}^n = O(\Delta t^2) \geq 0$
- Additional advantage: allows local time-stepping for slow-fast systems
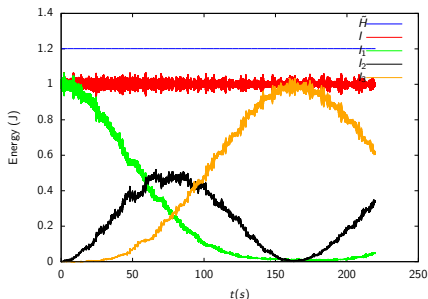
Bilbao's scheme

- Quadratization by introducing an auxiliary variable, same cost as Verlet
- Exact positive energy
- Conservation at half-steps
- Prioritize exact kinetic energy
- No control on q, only on ψ
- Requires lower bounded potential energy, dependent on the gauge
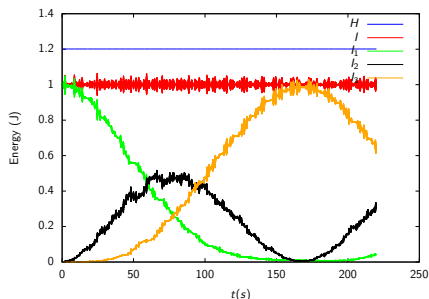- Allows arbitrary large time-steps

Numerical results: Fermi-Pasta-Ulam
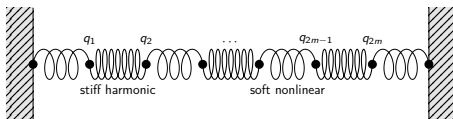
$$H(q,p) = \frac{1}{2}\sum_{i=1}^{m}(p_{2i-1}^2 + p_{2i}^2) + \frac{\omega^2}{4}\sum_{i=1}^{m}(q_{2i} - q_{2i-1})^2 + \sum_{i=0}^{m}(q_{2i+1} - q_{2i})^4$$

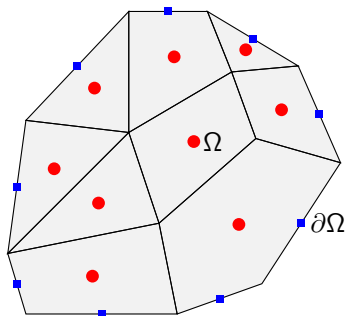
Energy variation, present scheme, $\Delta t = 10^{-3}$

Reference RK4 solution, $\Delta t = 10^{-4}$

Plan

Cell-Centered Galerkin scheme

- Similar to Finite Volume methods or lowest order DG [D. Di Pietro M2AN 2012]
- Works on general polyhedral meshes (simplices here)
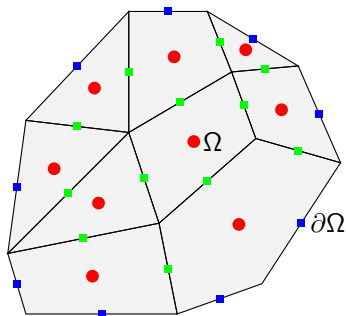- Displacement unknowns on cells and boundary faces

- $(u_c)_{c \in \mathcal{C}}$
- $(u_f)_{f \in \mathcal{F}^\partial}$

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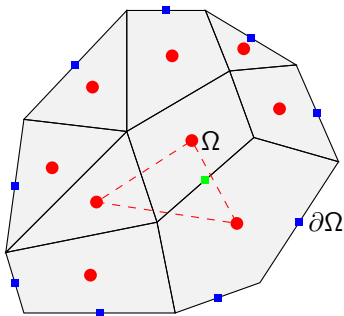- $(u_f)_{f \in \mathcal{F}^\partial}$
- $(u_f)_{f \in \mathcal{F}^i}$

Cell-Centered Galerkin scheme

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$$u_f = \sum_{c \in \mathcal{C}} \alpha_{fc} u_c$$

$$\sum_{c \in \mathcal{C}} \alpha_{fc} = 1$$

Ω

$\partial\Omega$

- $(u_c)_{c \in \mathcal{C}}$
- $(u_f)_{f \in \mathcal{F}^\partial}$
- $(u_f)_{f \in \mathcal{F}^i}$

Reconstructed gradient

- On each cell $c \in \mathcal{C}$:

$$G_c(v_\mathcal{F}) = \sum_{f \in \partial c} \frac{|f|}{|c|} v_f \otimes n_{f,c}$$

$$\varepsilon_c(v_\mathcal{F}) = \frac{1}{2}(G_c(v_\mathcal{F}) + G_c(v_\mathcal{F})^T)$$

- For elasticity, continuous weak form:

$$a(v, \tilde{v}) = \int_\Omega \varepsilon(v) : \mathbb{C} : \varepsilon(\tilde{v}),$$

$$\forall \tilde{v} \in V, \ \langle \rho \ddot{v}, \tilde{v}_h \rangle_{V',V} + a(v, \tilde{v}) = \int_\Omega f \tilde{v}.$$

- Discrete bilinear form: substitute reconstructed displacements on faces discrete gradients:

$$a_h(v_h, \tilde{v}_h) = \sum_{c \in \mathcal{C}} |c| \varepsilon_c(\mathcal{R}(v_h)) : \mathbb{C} : \varepsilon_c(\mathcal{R}(\tilde{v}_h))$$

Stabilization

- The scheme is not stable with only consistent terms.
- Local $\mathbb{P}_1$ displacement reconstruction on cell $c \in \mathcal{C}$:

$$\mathcal{I}_c(v_h, x) = v_c + G_c(\mathcal{R}(v_h)) \cdot (x - x_c).$$

- $\mathbb{P}_1$ reconstruction jump penalization on faces f:

$$[v_h]_f = \mathcal{I}_{c_1}(v_h, x_f) - \mathcal{I}_{c_2}(v_h, x_f)$$

$$s_h(v_h, \tilde{v}_h) = \sum_{f \in \mathcal{F}^i} |f| \frac{\eta}{h_f} [v_h]_f \cdot [\tilde{v}_h]_f$$

- Stabilization parameter η can be taken close to Young's modulus
- Complete discrete formulation:

$$\forall \tilde{v}_h \in V_h, \sum_{c \in \mathcal{C}} \rho |c| \ddot{v}_h \cdot \tilde{v}_h + a_h(v_h, \tilde{v}_h) + s_h(v_h, \tilde{v}_h) = \sum_{c \in \mathcal{C}} |c| f_c \tilde{v}_c.$$

Interpretation as a Discrete Element method (DEM)

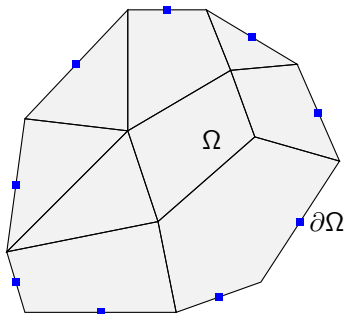- The discrete system follows a Hamiltonian dynamics with potential energy

$$\mathcal{E}_p(u_h) = \frac{1}{2} \left(a_h(u_h, u_h) + s_h(u_h, u_h) \right)$$

- Interactions between cell dofs (seen as rigid particles) can be expressed as forces:

$$F_c = -\nabla_{u_c} \mathcal{E}_p(u_h)$$

- Diagonal mass matrix
- The expression of force only involves the particle coefficients in the face reconstructions and normal stress jumps on faces.
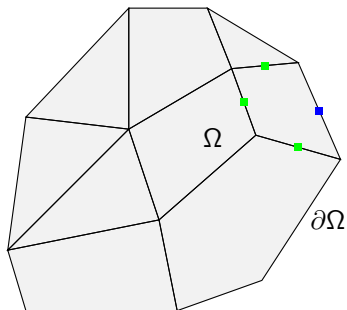
Boundary conditions

- Dirichlet BCs: impose u_f
- Neumann BCs: three possibilities

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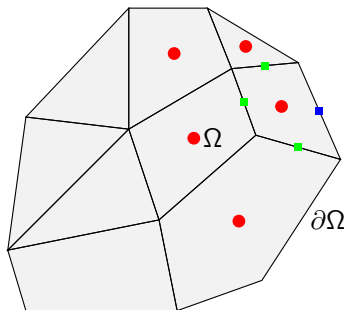
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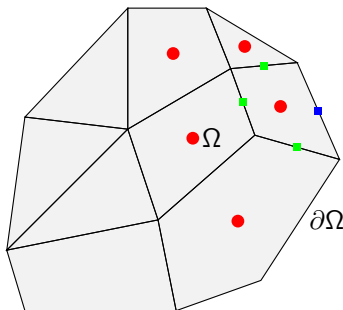- $(u_f)_{f \in \mathcal{F}^i}$

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- $(u_f)_{f \in \mathcal{F}^\partial}$
- $(u_f)_{f \in \mathcal{F}^i}$

- Dirichlet BCs: impose u_f
- Neumann BCs: three possibilities
  - Solve local problems $\sigma_c \cdot n_{f,c} = 0$
  - Extrapolate from close u_c
 - Take adjacent value u_c (loss of accuracy)

Contact

- Signorini-type problem
- Additional difficulties:
    - Possible contact between several faces at a time
    - Need a continuous reconstruction of the u_f from the u_c (conservation of energy)
- Compute face reconstructions u_f (without taking contact into account)
- Detect contact zones (potential contact)
- For two faces f_1 and f_2 face-to-face, if $(u_{f_2} - u_{f_1}) \cdot n_{f_1 f_2} \leq 0$, modify reconstruction:

$$\tilde{u}_{f_1} = u_{f_1} + \frac{|f_1 \cap f_2|}{2|f_1|}(u_{f_2} - u_{f_1}) \cdot n_{f_1 f_2} n_{f_1 f_2},$$
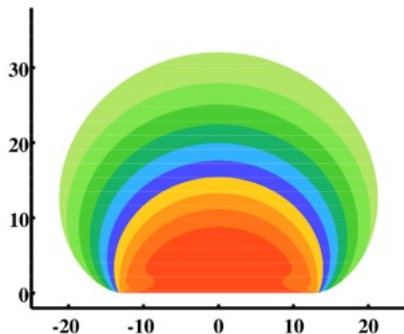
$$\tilde{u}_{f_2} = u_{f_2} + \frac{|f_1 \cap f_2|}{2|f_2|}(u_{f_1} - u_{f_2}) \cdot n_{f_1 f_2} n_{f_1 f_2}.$$

- Allows perfect slip on two discretized surfaces
- Impose non-penetration of massless dofs: see Khenous Laborde Renard 2008

Static validation: Hertz contact test-case
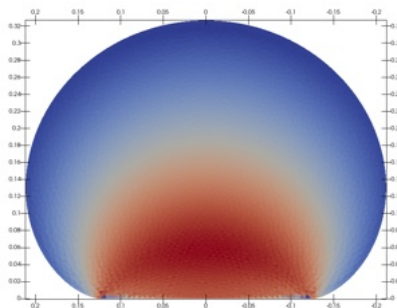
CCG result

FEM result with Nitsche's penalization [Chouly Hild Renard 2015]

- Static computation
- BFGS solver: no need for linear algebra, pseudo-inverse initialized as a diagonal matrix (Young's modulus inverse)

Nonlinearities

- Evaluate the force integral through numerical quadrature
- In the case of contact, increasing the quadrature order does not yield satisfactory results: nonsmooth function
- Modify quadrature: identify contact event times and carry out exact numerical quadrature on each time subinterval.
- No global time sub-cycling: detect locally contact events for face pairs and evaluate locally the additional quadrature points needed for force integration
- Allows to maintain exact energy conservation

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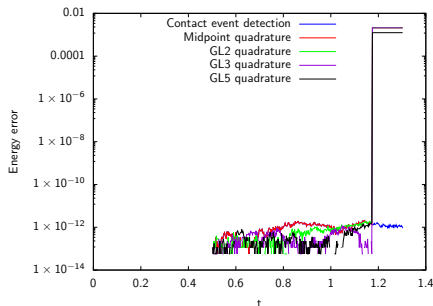
Cylinders rebound

Energy conservation
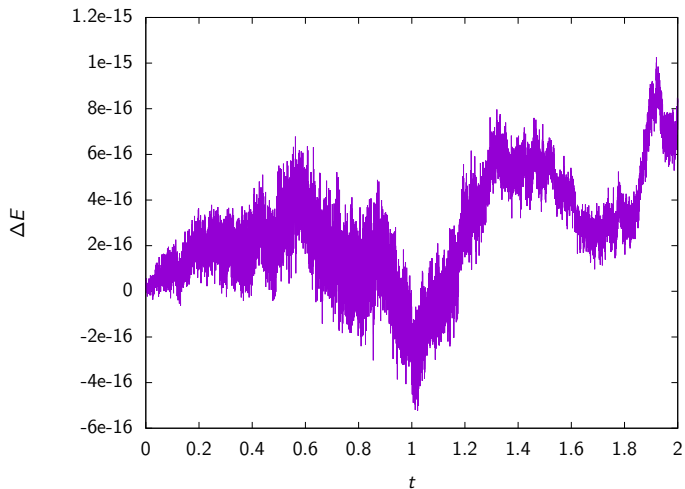
Slipping cylinders rebound

Billiard

Plan

Perspectives

- Time-integration scheme:
    - Extension to higher order?
- Space discretization:
    - Add friction laws in contact
    - Large deformation and corotational formulation
    - DG in space with contact?
    - Handle shock waves (regularization techniques by Clamond and Junca)

Thank you for your attention!

- References:
    - F. Marazzato, A. Ern, LM and C. Mariotti, An explicit pseudo-energy conserving time-integration scheme for Hamiltonian dynamics, *CMAME* 347:906-927, 2019.
    - F. Marazzato, A. Ern, LM, A variational discrete element method for quasistatic and dynamic elastoplasticity, *IJNME* 121:5295-5319, 2020.
    - N. Dirani, LM, An explicit pseudo-energy conservative scheme for contact between deformable solids, submitted, *HAL preprint* 03879345, 2022.