## Using Extended Interval Algebra in Discrete Mechanics

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- 1. Model a physical phenomenon using a differential equation (or a system of differential equations) or a variational principle
- 2. Obtain the algebraic forms of the differential equation(s) or variational principle by forcing them into the mold of discrete time and space
- 3. In order to commit to algorithms, project real-valued variables onto finite computer words => round-off & truncation

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Peraire and co-workers => Certificates for PDEs (certified bounds on discretization errors).

Elliptic problems, limit theory of plasticity, J-integral

Sauer-Budge, A.M., Bonet, J., Huerta, A., and Peraire, J., Computing bounds for linear functionals of exact weak solutions to Poisson's equation, *SIAM Journal on Numerical Analysis*, 42, 4 1610-1630, (2004).

Xuan, Z.C., Parés, N. and Peraire, J., Computing upper and lower bounds for the J-integral in two-dimensional linear elasticity. *Computer Meth. in Appl. Mech. and Engng.*, 195, 430-443 (2006).

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Interval Analysis and Reliable Computing

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## **VERIFICATION AND VALIDATION**

## CA approach to modeling physical systems

## **Physical System**



## **Physical system (computer)**

## CA approach to modeling physical systems



## Discrete Mechanics (Baez and Gilliam, 1994 & 1996)

- Time evolution proceeds in integer steps
- Configuration space is discrete
- Differential geometry => Algebraic geometry
- Euler-Lagrange Equation
- Noether theorem
- Symplectic techniques



Example of mechanical system
Introduce imprecision using extended intervals

Configuration space = ring k of rational numbers
Particle of mass m constrained to move on a line: q<sub>0</sub>, q<sub>1</sub>,...
Algebra A of functions on k:

$$A \cong k[q] = \left\{\lambda_0, \lambda_0 + \lambda_1 q, \lambda_0 + \lambda_2 q^2, \lambda_0 + \lambda_1 q + \lambda_2 q^2 : \lambda_0 + \lambda_3 q^3, \ldots\right\}$$

Lagrangian

$$A \otimes A \cong k[q_1, q_2] \quad \mathscr{L}_i = \mathscr{L}(q_i, q_{i+1}) = \frac{1}{2} m \dot{q}_i^2 - V(q_i) \quad \dot{q}_i = q_{i+1} - q_i$$
  
•Space of histories

$$H \cong k[q_0, ..., q_T]$$

Lagrange equation

$$d_i \mathscr{L}_i + d_i \mathscr{L}_{i-1} = 0$$
  $m(\dot{q}_i - \dot{q}_{i-1}) = -V'(q_i)$ 



m = 1  $q_0 = 8$   $q_1 = 16$   $V = \frac{1}{2Sq^2}$ s = 1

*{*8, 10, 56/3,  $m=1 \qquad 1\overline{36/9},$  $q_0 = 8$  176/27,  $q_1 = 16$  -344/81,  $V = \frac{1}{2}sq^2$  -3304/243, s/m = 1/3 -13424/729, -37384/2187, -66104/6561, 5936/19683, 624616/59049, 3069656/177147  $\ldots \}$ 



#### 100 time steps

#### 1,000 time steps

#### 10,000 time steps

# Integer coordinates?All coordinates?

#### •Maximum and minimum coordinates:

- 100 steps: [-18.68289250959053, 18.682435719981747]
- 1,000 steps: [-18.68289250959053, 18.683060458305423]
- 10,000 steps: [-18.683972612054987, 18.6839719940311]

•Configuration space = conditional ring *D* of ext. intervals •Particle of mass m constrained to move on a line:  $q_0$ ,  $q_1$ ,...

•Lagrangian

$$\mathscr{L}_{i} = \mathscr{L}\left(\mathbf{q}_{i}, \mathbf{q}_{i+1}\right) = \frac{1}{2}\mathbf{m}\mathbf{q}_{i}^{2} - \mathbf{V}\left(\mathbf{q}_{i}\right)_{-1}$$

Lagrange equation

$$Dual(d_i\mathscr{L}_i) + d_i\mathscr{L}_{i-1} = 0$$

$$(\mathbf{m}\dot{\mathbf{q}}_i) - \mathbf{m}\dot{\mathbf{q}}_{i-1} + \mathbf{V}'(\mathbf{q}_i) = 0$$

#### •Newton's law:

$$(\mathbf{m}\dot{\mathbf{q}}_{i})_{-} - \mathbf{m}\dot{\mathbf{q}}_{i-1} + \mathbf{V}'(\mathbf{q}_{i}) = 0 \Leftrightarrow (\mathbf{m}\dot{\mathbf{q}}_{i})_{-} = (\mathbf{m}\dot{\mathbf{q}}_{i-1})_{-} - \mathbf{V}'(\mathbf{q}_{i})_{-} \Leftrightarrow \dot{\mathbf{q}}_{i} = \dot{\mathbf{q}}_{i-1} - \mathbf{m}^{-1}\mathbf{V}'(\mathbf{q}_{i})_{-} \Leftrightarrow \dot{\mathbf{q}}_{i} = -\mathbf{m}^{-1}\mathbf{V}'(\mathbf{q}_{i})_{-} \Leftrightarrow \dot{\mathbf{q}}_{i} - \dot{\mathbf{q}}_{i-1} = -\mathbf{m}^{-1}\mathbf{V}'(\mathbf{q}_{i})_{-}$$

#### •Example:

 $\mathbf{q}_0 = [11, 000, 11, 100]$  $\mathbf{q}_1 = [10, 000, 11, 000]$ 

$$\mathbf{V}(\mathbf{q}_1) = \frac{1}{2} \mathbf{s} \mathbf{q}_1^2$$

s = [1/5000, 3/5500]m = [1, 2]

## Used Popva's algorithm (2005) to eliminate dependency in flow calculation

97840	109989
11	10
23547324	1099670011
3025	100000
27741730507	10993400549989
4159375	100000000
126999172635479	109890016499230011
22876562500	100000000000
557422553635612563	1098350384969200989989
125821093750000	1000000000000000
2288250850107591605311	10976907699076049498790011
692016015625000000	100000000000000000000000000000000000000
8301862351155904852855067	109692138576901814927401429989
380608808593750000000	100000000000000000000000000000000000000
22075992059906839606189421799	1096042309491854446854100098350011
2093348447265625000000000	100000000000000000000000000000000000000
8361651439670606649600705226397	10950536289837415589895004868001869989
115134164599609375000000000000	100000000000000000000000000000000000000
759751840694239559412888964794437809	109395544311273029696900192520168297910011
633237905297851562500000000000000	100000000000000000000000000000000000000
8102051036064516583713118612745923335573	1092747861697407761918806463410658791002309989
3482808479138183593750000000000000000	100000000000000000000000000000000000000
66115762062600742198853274199335175199046281	10914310054959154860924191209732935370254097470011
1915544663526000976562500000000000000000	100000000000000000000000000000000000000
481987991561468735303467618334524740762828702157	109000500619387361871742253662383095369480696402749989
105354956493930053710937500000000000000000000	100000000000000000000000000000000000000

-40000	-20000	0	20000	40000
-40000	-20000	<i>i</i> =1	20000	40000
40000	20000	<i>i</i> =20	20000	40000
-40000	-20000	0	20000	40000
		<i>i</i> =40		
-40000	-20000	<i>i</i> =60	20000	40000
-40000	-20000	0 <i>i</i> — <b>80</b>	20000	40000
10000	20000	<i>l</i> -80		40000
-40000	-20000	<i>i</i> =140	20000	40000
-40000	-20000	0 ;—160	20000	40000
		<i>l</i> =100		
-40000	-20000	₀ <i>i</i> =180	20000	40000
-40000	-20000	₀ <i>i</i> =200	20000	40000

## Conclusions

 It may be impossible to determine a priori the evolution of even the simplest discrete mechanical system (sit down and let it evolve)

•When the system takes values on the set of extended intervals:

1) Introduce "Dual" in Lagrange equation.

2) Exact bounds can be calculated for i-th time step (monotonicity, Popova 2005)

3) Taylor models for flow of non-monotonic time evolutions?

## Thanks

## Evgenija D. Popova (Institute of Mathematics and Informatics, Bulgarian Academy of Sciences)