# Data, Lagrangian, Action!

Simulating mechanisms direct from a text file

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# Summary

- ► We solve a mechanism directly from a Lagrangian form
  - We don't explicitly derive equations of motion
  - No symbolie algebra to manipulate equations
  - We work in cartesian coordinates
- Lagrangian derived from a text file description—the Data
- Action means the resulting animation
- Our technology is based on
  - Automatic differentiation (AD, aka algorithmic differentiation)
  - DAETS (NN, JP, 2009–), a C++ solver for high-index differential-algebraic equations (DAEs)
     Based on Pryce's structural analysis, and Taylor series

# System

- We have built a system that
  - Data: reads a text-file specification of a mechanism, initial conditions etc.
  - Creates Lagrangian; calls DAETS to solve and write output file
  - Action: visualizes by our MATLAB code animate3Dmech.m



 Text-file is in YAML, a human-readable data serialization language

### Outline

Example

Lagrangian mechanics

Lagrangian facility

Mechanism facility

More examples

Conclusion

# Example: Mechanism1

Lagrangians

- S uniform thin rods AC, BD, EF of mass m and length ℓ
- ► A uniform triangular (45°45°90°) plate CDE of mass M and short side ℓ
- Pin-jointed at C, D, E and at fixed points A, B on same horizontal level, distance L apart, from which system hangs
- Moves under gravity



#### Dramatis Personae (Mechanism 1 specification in YAML)

Title: Mechanism1 Dimension: 2 **PhysicalParams:** 

Lagrangians

1: 1 # length  $\ell$  of rods L: 0.58 # distance of top pivots A, B m: 2 # mass of rods M: 5 # mass of plate

#### PartData:

# coordinates of fixed points. **Fixed**: {A: [-L/2], B: [L/2]} Rigids:

*# Geom: local frame geometry* 

*#Dyna: centroid, mass, moment of inertia* 

AC, BD, EF: {Geom: [1]], Dyna: [1/2], m, m\*1\*\*2/12]} CDE:

```
Geom: [ [l*sqrt(2)], [l/sqrt(2), -l/sqrt(2)] ]
```

```
Dyna: [ [l/sqrt(2), -l/(3*sqrt(2))], M, M*l**2/9 ]
```

AppliedForces: Gravity:

#turns it on with default value in SI units

Act 1 Scene 1 + Stage Directions (IVs; solver & animation settings)

**ProblemData:** *# integration interval, etc.* t0: 0 tend: 60 # Guesses for  $C, \dot{C}$  etc. where "fixed" means IV not guess - don't change it positions: {C: [[-1/sqrt(2), fixed], -1], D: [1/sqrt(2), -1], F: [[0, fixed], -l\*(1+1/sqrt(2))]} velocities: {C: [[-6, fixed], 0], D: [2, 0], F: [[3, fixed], 0]} #That starts it in equilibrium position & gives a sideways "kick" **SolverParams** : *# to guide DAETS* Integration : tol: 1e-12 order: 20 **OutFile:** #says output 0th and & 1st derivative of each moving point points: [C: 2, D: 2, E: 2, F: 2] tformat: '%...17e' #to 17 sig figs gformat: '%...17e' **Animation**: *#this guides animate3Dmech.m* **view**: [0, 90] # camera azimuth, elevation Skeleton: zscale: 0.02 #vertical scale, e.g. of fixed pivots fleshoutwid: 0.05 #says how wide "thin" things are drawn

#### Lagrangian mechanics theory

The Lagrangian function

L = T - V

is a powerful way to describe a mechanical system

- ► T = total kinetic energy, in terms of velocities and possibly positions
- ► V = total potential energy, caused by conservative (energy preserving) forces depending only on system position
- May also have holonomic (not velocity-dependent) constraints on motion, and/or external applied forces
- Simplifies modelling!

#### Lagrangian cont.

- Describe configuration at time t by vector q = (q<sub>1</sub>,...,q<sub>n<sub>q</sub></sub>) of generalised position coordinates
- Vector q is generalised velocities
- Assumptions from previous slide imply

L = T - V, with  $T = T(\mathbf{q}, \dot{\mathbf{q}}), V = V(\mathbf{q})$ 

plus any constraints on motion:

 $0 = C_j(t, \mathbf{q}), \qquad j = 1: n_c$ 

Lagrangian cont.

Whatever coordinates chosen, variational "stationary action" principle gives (n<sub>q</sub>+n<sub>c</sub>) Euler-Lagrange equations of motion:

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} + \sum_{j=1}^{n_c} \lambda_j \frac{\partial C_j}{\partial q_i} = Q_i(t), \qquad i = 1: n_q \qquad (1)$$
$$C_j(t, \mathbf{q}) = 0, \qquad j = 1: n_c \qquad (2)$$

- λ<sub>j</sub> are Lagrange multipliers for the constraints Q<sub>i</sub>(t) are generalised external force components, if any (whose definition also involves ∂/∂q<sub>i</sub>)
- If  $n_c > 0$  the system is of first kind and is an index 3 DAE
- If  $n_c = 0$  the system is of second kind, reducible to an ODE

#### Example: free motion of simple pendulum

Taking  $\mathbf{q} = (x, y) = \text{cartesian coordinates of pendulum bob (of mass <math>m$ ) with y downward, gives

$$T = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2), \qquad V = -mgy$$
$$L = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) + mgy$$



with one constraint that we write

 $0 = C = \frac{1}{2}(x^2 + y^2 - \ell^2)$ 

Euler–Lagrange, on dividing through by m, give pendulum DAE

$$\begin{array}{ll}
0 = A &= \ddot{x} + x\lambda & \text{from } 0 = \frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} + \lambda \frac{\partial C}{\partial x} \\
0 = B &= \ddot{y} + y\lambda - g & \text{from } 0 = \frac{d}{dt}\frac{\partial L}{\partial \dot{y}} - \frac{\partial L}{\partial y} + \lambda \frac{\partial C}{\partial y} \\
0 = 2C &= x^2 + y^2 - \ell^2
\end{array}$$
(3)

#### Pendulum cont.

Alternatively, taking  $\mathbf{q}=(\theta)=$  angle of pendulum from downward vertical, gives

$$T = \frac{1}{2}m(\ell\dot{\theta})^2, \qquad V = -mg\ell\cos\theta$$
$$L = \frac{1}{2}m(\ell\dot{\theta})^2 + mg\ell\cos\theta$$

with no constraints. Then Euler-Lagrange lead to an ODE form

$$\ddot{\theta} = -\frac{g}{\ell}\sin\theta$$
 from  $0 = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial\dot{\theta}} - \frac{\partial L}{\partial\theta}$ 

which is equivalent to the DAE

For one pendulum the angle model wins, but for n > 1 pendula (in a chain) the cartesian model is **much** simpler ...

Example: n > 1 pendula, in 3D cartesians

- $\mathbf{r}_i = (x_i, y_i, z_i)$  position of *i*th bob (with *z* downward)
- Generalized coordinates

$$\mathbf{q} = (\mathbf{r}_1, \dots, \mathbf{r}_n) = (x_1, y_1, z_1, \dots, x_n, y_n, z_n)$$

1st kind formulation is

$$L = \frac{1}{2}m\sum_{i=1}^{n} |\dot{\mathbf{r}}_{i}|^{2} + mg\sum_{i=1}^{n} z_{i}$$

$$0 = C_{j} = |\mathbf{r}_{j} - \mathbf{r}_{j-1}|^{2} - \ell^{2}, \qquad j = 1:n$$
(4)

where  $\mathbf{r}_0 = \mathbf{0}$ , and  $|\cdot|^2$  is the squared length of a 3-vector

- Constraints say the rods have length  $\ell$
- ▶ 3n coordinate variables, n Lagrange multipliers Hence second-order DAE of size 4n and index 3
- ▶ DAETS with our "Lagrangian facility" solves (4) as written

#### Example: The same, in ODE form

- $\blacktriangleright$  Use spherical polar coordinates  $(\theta_i,\phi_i)$  for rod i
  - $\theta_i$  is rod's angle with downward vertical
  - $\phi_i$  is angle of rotation from the xz plane
- With  $\mathbf{q} = (\theta_1, \phi_1, \dots, \theta_n, \phi_n)$  we can get rid of the constraints
- $\blacktriangleright~2n$  coordinates, so 4n ODEs when reduced to first-order
- Formulation is way more complex. E.g. KE is

$$T = \frac{1}{2}m\ell^2 \sum_{k=1}^n \left| \sum_{i=1}^k \left( \cos\theta_i \,\dot{\theta}_i \cos\phi_i - \sin\theta_i \sin\phi_i \,\dot{\phi}_i \\ \cos\theta_i \,\dot{\theta}_i \sin\phi_i + \sin\theta_i \cos\phi_i \,\dot{\phi}_i \\ -\sin\phi_i \,\dot{\phi}_i \end{array} \right) \right|^2$$

and you still have the  $\partial/\partial q_i, \partial/\partial \dot{q}_i$  stuff to do

 It seems any other way to remove the constraints will use angles in some form

#### Summary advantages of a high-index DAE code

- Index measures how difficult is to solve a DAE compared to an ODE (index 0)
- ODEs and index-1 DAEs seen as "easy" to solve and highindex DAEs as "hard"
- So considerable effort is spent to find coordinates giving a 2nd-kind Lagrangian and deriving equations of motion
- But mathematical model often simpler in cartesian coordinates
- ► DAETS handles resulting 1st kind Lagrangian systems easily
- We streamline this by DAETS's Lagrangian facility and mechanism facility ...

#### First... Lagrangian facility

- On top of DAETS, this solves directly from L and the constraints
  - ▶ Builds on AD package FADBAD++ which is integral to DAETS
  - Computes derivatives "on the fly" behind the scenes
  - No symbolic algebra
- Very efficient (thanks to Xiao Li, M.Sc. McMaster U)
  - common subexpression elimination through operator overloading in AD
  - sparse algorithms in AD
  - sparse linear algebra

#### Next... mechanism facility

Lagrangians

Building on the previous, our goal is to

- 1. *Theory*: Express Lagrangian of mechanism (robot arm etc.) by x, y, z coordinates of chosen reference points (RPs) on its parts
  - In 2D, a rigid body's position is fixed by 2 points on it in "general position"; in 3D, by 3 points; etc
  - Express its PE (if relevant) and KE in terms of world-positions and velocities of such RPs
  - Hence multi-body  $L = L(\mathbf{q}, \dot{\mathbf{q}})$  with  $\mathbf{q} = (\text{suitable RPs})$
  - ▶ ...entirely in cartesian coordinates
- 2. Practice: Create
  - text file syntax/semantics for describing a class of mechanisms
  - C++ API to convert this to a Lagrangian that DAETS then handles by the Lagrangian facility

#### What mechanism facility currently provides

We are tidying up 2D before moving to 3D

- Named Points; same point on two parts means joined there
  - One declares some points fixed in world frame
  - All others are assumed moving
- Parts (a part's name is the list of points on it)
  - Rigid body (dynamics = mass, centroid, moment of inertia)
  - Particle (dynamics = mass only)
  - Spring (dynamics = stiffness, rest-length) Optionally mass, then dynamics of a stretchable uniform rod
- Forces
  - Constant (in world frame or in local frame) force
     Applied at a named point of body, fixed in local frame
  - Constant torque on a rigid part
  - Time-varying forces still to come—need compile/link stage
- Collinears
  - Constrains 3 or more points to lie on a straight line Useful for specifying various kinds of joint

### Mechanism2

- Rigid rods CK, KM, DL, LM, EF, FP and triangle plate CDE
- ▶ Springs AC, BD
- Point masses at M, N, P
- Collinear G, H, P

Animation





- Part of MBS Multi-Body Systems Benchmark in OpenSim
- Also in the Test Set for IVP Solvers, where ....
  - It is formulated as an index 3 DAE in angle coordinates
  - Equations are not pretty at all
- We modeled and solved in cartesian coordinates
- Confirmed very close agreement between the two solutions



#### Further examples

- These are in 3D so don't use the mechanism facility, but do use the Lagrangian facility
- John P extended the basic rigid body reference point theory to 3D and we are working out the implications
- Indeed we can do rigid body dynamics in any dimension
- QR factorization is key to the algorithm No quaternions
- Example: multi-pendulum made of genuinely 3D rods joined by Universal Joints (Hooke–Cardan joints)
   UJs transmit torque round a bend—permit 2 DOF of relative angular position but forbid relative rotation about rod-axes



#### Larger example: Particle-spring system

 Rectangular grid of *m* × *n* particles connected by damped springs

Lagrangians

 A test for cloth simulation in movies



• Particle (i, j) is attached to

$$(i \pm 1, j)$$
 and  $(i, j \pm 1)$  for  $i = 1 : m, j = 1 : n$ 

► Index i = 0 or m + 1, resp. j = 0 or n + 1, means a fixed position

## Particle-spring cont.

Lagrangians

- ► Each particle (*i*, *j*)
  - ▶ coordinates  $m{r}_{ij} = \left(x_{ij}, y_{ij}, z_{ij}\right)$  full 3D motion
  - $\blacktriangleright \ {\rm mass} \ M$
- Each spring
  - ► stiffness k
  - length at rest l
  - damping  $k_d \times$  stretch-rate (except the boundary ones)
- Spacing  $\Delta x$  and  $\Delta y$  between particles in x and y directions
- Initially all particles at rest in xy plane, we push the middle particle upwards
- ▶  $90 \times 90$  particles,  $24\,300$  second-order ODEs



# Particle-spring cont

Lagrangian is

$$L = \frac{1}{2}M\sum_{i=1}^{m}\sum_{j=1}^{n}|\dot{\boldsymbol{r}}_{ij}|^2 - Mg\sum_{i=1}^{m}\sum_{j=1}^{n}z_{ij}$$
$$-\frac{1}{2}k\left[\sum_{i=1}^{m}\sum_{j=0}^{n}(|\boldsymbol{r}_{i,j+1} - \boldsymbol{r}_{ij}| - l)^2 + \sum_{j=1}^{n}\sum_{i=0}^{m}(|\boldsymbol{r}_{i+1,j} - \boldsymbol{r}_{ij}| - l)^2\right]$$

We use Rayleigh's dissipative function

$$R = \frac{1}{2}k_d \sum_{i=1}^{m} \sum_{j=1}^{n-1} |\dot{\mathbf{r}}_{i,j+1} - \dot{\mathbf{r}}_{ij}|^2 + \frac{1}{2}k_d \sum_{j=1}^{n} \sum_{i=1}^{m} |\dot{\mathbf{r}}_{i+1,j} - \dot{\mathbf{r}}_{ij}|^2$$

- We encode L and R—that's all
- DAETS solves a sparse, second-order ODE of size  $3 \cdot m \cdot n$

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{\boldsymbol{r}}_{ij}} - \frac{\partial L}{\partial \boldsymbol{r}_{ij}} + \frac{\partial R}{\partial \dot{\boldsymbol{r}}_{ij}} = 0, \qquad i = 1:m, \ j = 1:n$$

# Conclusions and further work

Lagrangians

- "Data, Lagrangian, Action" works as a practical tool.
   We aim now to develop 3D, and improve user interface
- An implication for teaching the subject:
  - Since high-index DAEs are now as easy to solve as ODEs, a Lagrangian formulation needn't avoid constraints
  - So rigid-body mechanical systems can be modeled in cartesian coordinates, which is simpler
  - This makes the concept so easy that Lagrangian stuff can be taught at undergraduate level
     After doing some simple cases from first principles, students can experiment with a tool like the mechanism facility
- But there's a big new thing for Ned & me to learn ...

#### The natural coordinates community

Ned & I have only recently learnt of work going on for  $\sim 30$  years, on multi-body modelling by "natural coordinates"

- ▶ Their basic object is the rigid-body shift+rotate map  $\mathcal{R} \mapsto \mathbf{p}(t) + Q(t)\mathcal{R}$  stored as  $3 + 3 \times 3 = 12$  scalars per body
- ► Our basic object is point x(t). In 3D, three points define body position, making 3 × 3 = 9 scalars per body (less, as points are shared)
- They mostly have Finite Elements background so very different mind-set from ours.
  - Tasks considered serious but  $\operatorname{DAETS}$  probably handles well:
    - Finding e.g. equilibrium configuration
    - Analysis of kinematic chains

#### References

- JP, NN, G. Tan, X. Li. How AD can help solve differentialalgebraic equations
   Optimization Methods and Software, 2018, DOI
- ▶ JP, NN. Write-up of this as a paper, same title We are wondering where to submit it to.
- YouTube channel Multi-body Lagrangian Simulations
  - Outer planets
  - Gravitating masses in 2D
  - Spring mass with 3 pendula
  - ▶ ..

#### Appendix: YAML text for Andrews squeezing mechanism

Complete description except for PhysicalParams values and Title. The boxed text specifies the topology, geometry and dynamics.

```
Dimension: 2
PartData:
Fixed: {0: [], A: [xa, ya ], B: [xb, yb], C: [ xc, yc] }
Rigida:
OF: { Geon: [ [rr] ], Dyna: [ [ ra ], mi, 11 ] }
FE: { Geon: [ [ra] ], Dyna: [ [ ra ], mi, 12 ] }
ED: { Geon: [ [ra] ], Dyna: [ [ ra ], mi, 14 ] }
AG: { Geon: [ [ra] ], Dyna: [ [ ra ], mi, 14 ] }
AG: { Geon: [ [ra] ], Dyna: [ [ ra ], mi, 15 ] }
HE: { Geon: [ [ra] ], Dyna: [ [ ra , b], mi, 15 ] }
HE: { Geon: [ [ra] ], Dyna: [ [ ra , ra], mi, 17 ] }
Spring:
CD: [ c0, 10 ]
AppliedForces:
Constrorques: { OF: mom }
```

Problempara: to: 0.0 tend: 0.03 positions: E: [-2e-02, 1e-03] F: [rr+cos(beta0), [rr+sin(beta0),fixed]] G: [-3e-02, 1e-02] H: [-3e-02, 1e-02] H: [-3e-02, 1e-02]

```
SolverParams:
 Mode: solve
 Integration:
  tol: 1e-14
  order: 17
 Display:
   tableau: false
   TVo. fales
  consIVs: false
   solution: false
   stats: false
   progress: false
 OutFile:
  tformat: '% .17e'
   gformat: '% .17e'
   points: [ D: 2, E: 2, F: 2, G: 2, H: 2 ]
   angles: [ OF: 1 ]
Animation:
 view: [-5, 27]
 physParamsToShow: [$beta0, $c0, $mom]
 Skeleton:
   zscale: 0.0005
   fleshoutwid: 0.0015
   Skels:
    BED: {path: XBXEXDX, newpts: [ X , [sa, sb] ] }
    AG: {path: YAYGY, newpts: [ Y , [ta, tb] ] }
```

```
AH: {path: ZHZAZ, newpts: [ Z , [ua, -ub] ] }
```