# Lights, Camera, 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 symbolic atgebra 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

- 3 uniform thin rods $A C, B D, E F$ of mass $m$ and length $\ell$
- A uniform triangular $\left(45^{\circ} 45^{\circ} 90^{\circ}\right)$ plate $C D E$ of mass $M$ and short side $\ell$
- 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
$\rightarrow$ Animation


## Dramatis Personae (Mechanism 1 specification in YAML)

Title: Mechanism1
Dimension: 2
PhysicalParams:
1: 1 \# length $\ell$ of rods
$\mathrm{L}: 0.58$ \# distance of top pivots $A, B$
$\mathrm{m}: 2$ \# 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: [ [l] ], Dyna: [ [l/2], m, m*l**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: $\quad 0$
tend: 60
\# Guesses for $C, \dot{C}$ etc. where "fixed" means IV not guess - don't change it positions: \{C: [[-1/sqrt(2), fixed],-l], D: [1/sqrt(2),-1], F: [ [0, fixed], $-1 *(1+1 / \operatorname{sqrt}(2))]\}$
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: $1 \mathrm{e}-12$
order: 20
OutFile: \#says output Oth and \& 1st derivative of each moving point points: [C: 2, D: 2, E: 2, F: 2]
tformat: ' ${ }^{\circ}$ п. $.17 \mathrm{e}^{\prime}$ \#to 17 sig figs qformat: ${ }^{\circ} \% .17 e^{\prime}$
Animation: \#this guides animate3Dmech.m
view: [0, 90] \# camera azimuth, elevation
Skeleton:
zscale: $\quad 0.02$ \#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 $\mathbf{q}=\left(q_{1}, \ldots, q_{n_{q}}\right)$ of generalised position coordinates
- Vector $\dot{\mathbf{q}}$ is generalised velocities
- Assumptions from previous slide imply

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

plus any constraints on motion:

$$
0=C_{j}(t, \mathbf{q}), \quad j=1: n_{c}
$$

## Lagrangian cont.

- Whatever coordinates chosen, variational "stationary action" principle gives $\left(n_{q}+n_{c}\right)$ Euler-Lagrange equations of motion:

$$
\begin{align*}
\frac{\mathrm{d}}{\mathrm{~d} t} \frac{\partial L}{\partial \dot{q}_{i}}-\frac{\partial L}{\partial q_{i}}+\sum_{j=1}^{n_{c}} \lambda_{j} \frac{\partial C_{j}}{\partial q_{i}} & =Q_{i}(t), & & i=1: n_{q}  \tag{1}\\
C_{j}(t, \mathbf{q}) & =0, & & j=1: n_{c} \tag{2}
\end{align*}
$$

- $\lambda_{j}$ are Lagrange multipliers for the constraints
$Q_{i}(t)$ are generalised external force components, if any (whose definition also involves $\partial / \partial q_{i}$ )
- 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 $\mathbf{q}=(x, y)=$ cartesian coordinates of pendulum bob (of mass $m$ ) with $y$ downward, gives

$$
\begin{aligned}
& T=\frac{1}{2} m\left(\dot{x}^{2}+\dot{y}^{2}\right), \quad V=-m g y \\
& L=\frac{1}{2} m\left(\dot{x}^{2}+\dot{y}^{2}\right)+m g y
\end{aligned}
$$


with one constraint that we write

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

Euler-Lagrange, on dividing through by $m$, give pendulum DAE

$$
\left.\begin{array}{lll}
0=A & =\ddot{x}+x \lambda & \text { from } 0=\frac{\mathrm{d}}{\mathrm{~d} t} \frac{\partial L}{\partial \dot{x}}-\frac{\partial L}{\partial x}+\lambda \frac{\partial C}{\partial x} \\
0=B & =\ddot{y}+y \lambda-g & \text { from } 0=\frac{\mathrm{d}}{\mathrm{~d} t} \frac{\partial L}{\partial \dot{y}}-\frac{\partial L}{\partial y}+\lambda \frac{\partial C}{\partial y} \\
0=2 C=x^{2}+y^{2}-\ell^{2} &
\end{array}\right\}
$$

## Pendulum cont.

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

$$
\begin{aligned}
& T=\frac{1}{2} m(\ell \dot{\theta})^{2}, \quad V=-m g \ell \cos \theta \\
& L=\frac{1}{2} m(\ell \dot{\theta})^{2}+m g \ell \cos \theta
\end{aligned}
$$

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

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

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

- $\mathbf{r}_{i}=\left(x_{i}, y_{i}, z_{i}\right)$ position of $i$ th bob (with $z$ downward)
- Generalized coordinates

$$
\mathbf{q}=\left(\mathbf{r}_{1}, \ldots, \mathbf{r}_{n}\right)=\left(x_{1}, y_{1}, z_{1}, \ldots, x_{n}, y_{n}, z_{n}\right)
$$

- 1st kind formulation is

$$
\left.\begin{array}{rl}
L & =\frac{1}{2} m \sum_{i=1}^{n}\left|\dot{\mathbf{r}}_{i}\right|^{2}+m g \sum_{i=1}^{n} z_{i}  \tag{4}\\
\\
C_{j} & =\left|\mathbf{r}_{j}-\mathbf{r}_{j-1}\right|^{2}-\ell^{2}, \quad j=1: n
\end{array}\right\}
$$

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

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


## Example: The same, in ODE form

- Use spherical polar coordinates $\left(\theta_{i}, \phi_{i}\right)$ for rod $i$
- $\theta_{i}$ is rod's angle with downward vertical
- $\phi_{i}$ is angle of rotation from the $x z$ plane
- With $\mathbf{q}=\left(\theta_{1}, \phi_{1}, \ldots, \theta_{n}, \phi_{n}\right)$ we can get rid of the constraints
- $2 n$ coordinates, so $4 n$ ODEs when reduced to first-order
- Formulation is way more complex. E.g. KE is

$$
T=\frac{1}{2} m \ell^{2} \sum_{k=1}^{n}\left|\sum_{i=1}^{k}\left(\begin{array}{c}
\cos \theta_{i} \dot{\theta}_{i} \cos \phi_{i}-\sin \theta_{i} \sin \phi_{i} \dot{\phi}_{i} \\
\cos \theta_{i} \dot{\theta}_{i} \sin \phi_{i}+\sin \theta_{i} \cos \phi_{i} \dot{\phi}_{i} \\
-\sin \phi_{i} \dot{\phi}_{i}
\end{array}\right)\right|^{2}
$$

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

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 $\mathbf{q}=$ (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 $C K, K M$, $D L, L M, E F, F P$ and triangle plate $C D E$
- Springs $A C, B D$
- Point masses at $M, N, P$
- Collinear $G, H, P$
- Animation



## Andrews squeezing mechanism



The original diagram. K3 is star-shaped and K 5 , K7 are not straight!


Fig. 9.1. Seven body mechanism (Schiehlen 1990, with permission)

- 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
$\rightarrow$ Animation


## 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
$\rightarrow$ Animation


## Larger example: Particle-spring system

- Rectangular grid of $m \times n$ particles connected by damped springs
- A test for cloth simulation in movies

- Particle $(i, j)$ is attached to

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

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


## Particle-spring cont.

- Each particle $(i, j)$
- coordinates $\boldsymbol{r}_{i j}=\left(x_{i j}, y_{i j}, z_{i j}\right)$ full 3D motion
- 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 $x y$ plane, we push the middle particle upwards
- $90 \times 90$ particles, 24300 second-order ODEs
- Animation


## Particle-spring cont

- Lagrangian is

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

- We use Rayleigh's dissipative function

$$
R=\frac{1}{2} k_{d} \sum_{i=1}^{m} \sum_{j=1}^{n-1}\left|\dot{\boldsymbol{r}}_{i, j+1}-\dot{\boldsymbol{r}}_{i j}\right|^{2}+\frac{1}{2} k_{d} \sum_{j=1}^{n} \sum_{i=1}^{m}\left|\dot{\boldsymbol{r}}_{i+1, j}-\dot{\boldsymbol{r}}_{i j}\right|^{2}
$$

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

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

## Conclusions and further work

- "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 $\mathbf{x}(t)$. In 3D, three points define body position, making $3 \times 3=9$ 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 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: { O: [], A: [xa, ya ], B: [xb, yb], C: [ xc, yc] }
    Rigids:
        OF: {Geom: [ [rr] ], Dyna: [ [ ra ],ml, il ] }
        FE: { Geom: [ [d ] ], Dyna: [ [ da ], m2, i2 ] }
        BED: (Geom: [ [ss], [sc, sd] ], Dyna: [ [sa, sb], m3, i3 ])
        EG: { Geom: [ [e] ], Dyna: [ [ea ], m4, i4 ] }
        AG: { Geom: [ [zt] ], Dyna: [ [ta, tb], m5, i5 ] }
        HE: {Geom: [ [zf] ], Dyna: [ [zf-fa], m6, i6 ] }
        AH: {Geom: [ [u] ], Dyna: [ [ua, -ub], m7, i] ] }
    Springs:
        CD: [ c0, 10]
AppliedForces:
    ConstTorques: { OF: mom }
```

```
ProblemData:
    t0: 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]
    velocities: # all 0's by default
```

```
SolverParams:
    Mode: solve
    Integration:
        tol: 1e-14
        order: 17
    Display:
        tableau: false
        IVs: false
        consIVs: false
        solution: false
        stats: false
        progress: false
    OutFile:
        tformat: '% .17e'
        qformat: '% .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] ] }
```

