

Modeling and Simulation of Lagrangian Mechanics through Automatic Differentiation and High-Index DAE Solving

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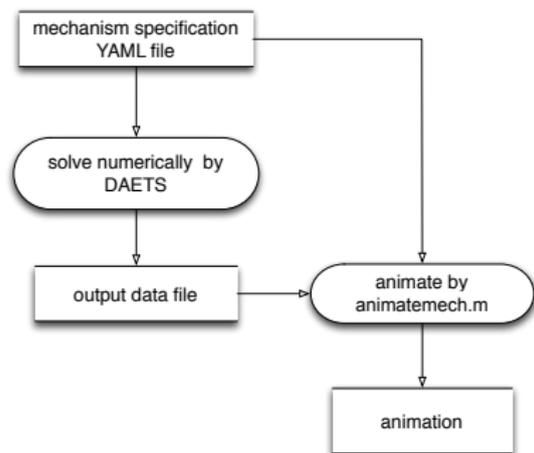
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Introduction

- ▶ A multi-body system or **mechanism** is made of rigid parts, springs etc., connected by joints, moving under various forces.
- ▶ John & I realized our high-index differential-algebraic equation (DAE) solver **DAETS** is well suited to simulating mechanisms.
- ▶ On top of DAETS we built a **Lagrangian facility**.
 - ▶ Using automatic differentiation (AD), from a Lagrangian function, constraints, . . . , it constructs at runtime Euler-Lagrange equations, an index-3 DAE, which DAETS integrates.
- ▶ We re-invented—differently—the ~ 30 years established **Natural Coordinates** (NCs) approach.
- ▶ **Mechanism facility** (in progress)
 - ▶ reads text-file spec of mechanism, initial values (IVs) etc.
 - ▶ assembles Lagrangian, constraints, ...

System “Data, Lagrangian, Action”

- ▶ **Data**: reads text-file spec of mechanism, IVs etc.
- ▶ Creates **Lagrangian**; calls **DAETS** to solve and write output file
- ▶ **Action**: visualizes by our **MATLAB** code **animatemech**



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

Examples

“Mechanism1”: [▶ Animate](#)

Andrews Mechanism: [▶ Animate](#)

Outline

DAETS solver

Lagrangian mechanics and using DAETS on it

Rigid body tracking

Example: the RSCR mechanism

Conclusion

References

More examples

DAETS overview

- ▶ DAETS— **D**ifferential **A**lgebraic **E**quations by **T**aylor **S**eries
- ▶ Solves DAE initial value problems, for state variables $x_j(t)$, $j = 1:n$, of the general form

$$f_i(t, \text{the } x_j \text{ and derivatives of them}) = 0, \quad i = 1:n.$$

- ▶ Can be **fully implicit**.
- ▶ **d/dt can appear anywhere** in the expressions for f_i
e.g. one of the equations could be

$$\frac{((x'_1 \sin t)')^2}{1 + (x'_2)^2} + t^2 \cos x_2 = 0.$$

DAETS's numerical method

- ▶ For some DAE with n equations $f_i = 0$ in terms of n variables $x_j(t)$ & their derivatives, define signature matrix $\Sigma = (\sigma_{ij})$

$$\sigma_{ij} = \begin{cases} \text{highest order of derivative of } x_j \text{ occurring in } f_i \\ \text{or } -\infty \text{ if doesn't occur.} \end{cases}$$

- ▶ Structural analysis (SA) derives non-negative integer offsets: c_1, \dots, c_n of the equations; d_1, \dots, d_n of the variables.
- ▶ Form system Jacobian $\mathbf{J} = (J_{ij})$ where

$$J_{ij} = \frac{\partial f_i}{\partial x_j^{(d_j - c_i)}}, \quad \text{or 0 where this makes no sense.}$$

$(x^{(p)} = p\text{th time derivative of } x.)$

- ▶ Mathematically (for smooth f_i)
 method succeeds at $\mathbf{x} \iff \mathbf{J}$ nonsingular at \mathbf{x}
 where “succeeds” = “generates Taylor series of solution at \mathbf{x} ”.

DAETS solves high-index problems

- ▶ Index ν measures how difficult is to solve a DAE compared to an ODE (index 0).
- ▶ For traditional methods, $\nu \geq 3$ considered hard.
- ▶ Based on **structural analysis** of DAE + **Taylor series**.
 - ▶ Builds on AD package **FADBAD++**.
- ▶ In principle unaffected by index.
- ▶ Finding consistent initial point is done through **IPOPT**, “software library for large scale nonlinear optimization”.

Lagrangian mechanics

- ▶ Lagrangian method is popular because it simplifies modeling.
 - ▶ Many ways to choose coordinates; all describe same motion.
- ▶ Lagrangian function

$$\mathcal{L} = T - V$$

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.

- ▶ Usually have **constraints** on motion—assume holonomic (velocity-independent) for simplicity—and external **forces**.

Lagrangian cont.

- ▶ Describe configuration at time t by vector $\mathbf{q} = (q_1, \dots, q_{n_q})$ of n_q **generalized position coordinates**.
 $\dot{\mathbf{q}}$ is **generalized velocities**.
- ▶ Assumptions from previous slide imply

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

plus n_c constraints on motion:

$$0 = C_i(t, \mathbf{q}), \quad i = 1 : n_c$$

- ▶ Assuming the C_j are independent, the system has

$$\text{DOF} = n_q - n_c \quad \text{positional } \text{degrees of freedom}.$$

Fix DOF q_j 's and DOF \dot{q}_j 's to specify an initial value problem.

Lagrangian cont.

- ▶ Whatever coordinates chosen, variational “stationary action” principle gives (n_q+n_c) **Euler–Lagrange equations** of motion:

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{q}_j} - \frac{\partial \mathcal{L}}{\partial q_j} + \sum_{i=1}^{n_c} \lambda_i \frac{\partial C_i}{\partial q_j} = Q_j(t), \quad j = 1:n_q \quad (1)$$

$$C_i(t, \mathbf{q}) = 0, \quad i = 1:n_c \quad (2)$$

- ▶ λ_i are **Lagrange multipliers** for the constraints.
 $Q_j(t)$ are **generalized external force** components, if any (whose definition also involves $\partial/\partial q_j$).
- ▶ If $n_c = 0$ the system is **of second kind**, reducible to an ODE.
 If $n_c > 0$ it's **of first kind** and is an index 3 DAE.

Example: free motion of simple pendulum

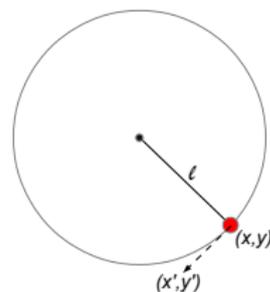
Taking $\mathbf{q} = (x, y) =$ Cartesian coordinates of pendulum bob (of mass m) with y downward, gives

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

$$\mathcal{L} = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) + mgy,$$

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 index-3 DAE

$$0 = A = \ddot{x} + \lambda x \quad \text{from } 0 = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}} - \frac{\partial \mathcal{L}}{\partial x} + \lambda \frac{\partial C}{\partial x}$$

$$0 = B = \ddot{y} + \lambda y - g \quad \text{from } 0 = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{y}} - \frac{\partial \mathcal{L}}{\partial y} + \lambda \frac{\partial C}{\partial y}$$

$$0 = 2C = x^2 + y^2 - \ell^2$$

Example: how Lagrangian facility works

- ▶ User encodes

$$\begin{aligned}\mathcal{L} &= \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) + mgy \\ C &= x^2 + y^2 - \ell^2\end{aligned}\tag{3}$$

- ▶ Lagrangian facility converts (3) to

$$\begin{aligned}0 &= m\ddot{x} + 2x\lambda \\ 0 &= m\ddot{y} + 2y\lambda - mg \\ 0 &= x^2 + y^2 - \ell^2\end{aligned}$$

which is of the form DAETS accepts.

Pendulum cont.

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

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

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

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

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

$$\left. \begin{aligned} \mathcal{L} &= \frac{1}{2}m \sum_{i=1}^n |\dot{\mathbf{r}}_i|^2 + mg \sum_{i=1}^n z_i \\ 0 &= C_j = |\mathbf{r}_j - \mathbf{r}_{j-1}|^2 - \ell^2, \quad j = 1:n \end{aligned} \right\} \quad (4)$$

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

- ▶ Constraints say the rods have length ℓ
- ▶ $3n$ 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

- ▶ Use spherical polar coordinates (θ_i, ϕ_i) for rod i
 - ▶ θ_i is rod's angle with downward vertical
 - ▶ ϕ_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.
- ▶ $2n$ coordinates, so $4n$ ODEs when reduced to first-order.
- ▶ Formulation is way more complex. E.g. KE is

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

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.

Choices

Independent coordinates $n_c=0$

- Often most of the coordinates are angles.
- Eqns reduce to ODE, but messy.
- “ODEs are nice to solve.”
- Has become a big industry with some elegant maths.

Dependent coordinates $n_c>0$

NCs use Cartesian coordinates of points fixed on bodies.
Eqns are index-3 DAE but simple.
“DAEs are nasty to solve.”
NCs are a smaller industry, also with some nice maths.

DAETS is well suited to DAEs of the NCs kind (assume smooth).

- ▶ Based on **structural analysis** SA of the DAE.
Theorem: SA “succeeds” on any DAE of this kind.
- ▶ Uses **Taylor series** of high order—typically 15–20.
- ▶ Infrastructure: **IPOPT** and **FADBAD++**.

Infrastructure benefits

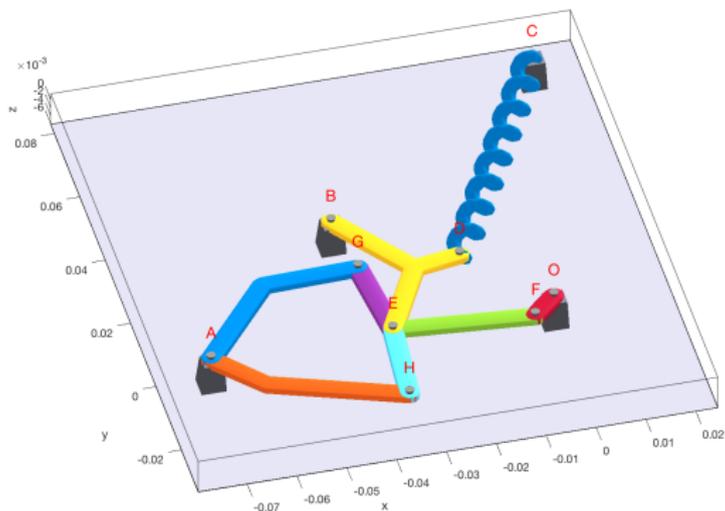
FADBAD++

- ▶ Inside DAETS forms **Taylor series** of solution, and **system Jacobian**.
- ▶ Outside DAETS, for a mechanism, **forms Euler–Lagrange DAE from \mathcal{L}** and constraints by doing $\partial/\partial\mathbf{q}$, $\partial/\partial\dot{\mathbf{q}}$ and d/dt at run time.

IPOPT

- ▶ Used by DAETS to find **initial consistent point** of DAE.
- ▶ For a mechanism this is initial position after fixing DOF IVs. IPOPT has proved very robust at finding this.
- ▶ Multiple solutions typical so need both **fixed IVs & guesses**.

E.g. in this Andrews Mechanism, G , H (independently) can lie either side of line AE .



How rigid motion is tracked

- ▶ Rigid motion of body \mathcal{R} is described by “shift & rotate” map

$$\mathcal{R}_t = \mathbf{O}_t + \mathbf{Q}_t \mathcal{R}, \quad \mathcal{R}_t \text{ is short for } \mathcal{R}(t), \text{ etc.} \quad (*)$$

\mathcal{R} : fixed in local frame

\mathcal{R}_t : moving in world frame WF

\mathbf{O}_t : WF position of \mathcal{R} 's moving local origin

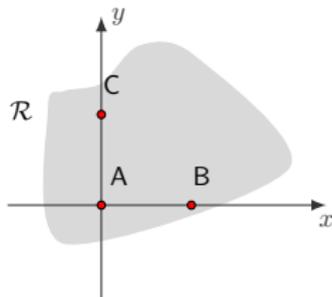
\mathbf{Q}_t : rotation, whose columns $[\mathbf{i}_t, \mathbf{j}_t, \mathbf{k}_t]$ are \mathcal{R} 's moving orthonormal basis (ONB)

- ▶ (*) means that any **point** X and **vector** \mathbf{u} fixed in \mathcal{R} move in the WF according to

$$X_t = \mathbf{O}_t + \mathbf{Q}_t X, \quad \mathbf{u}_t = \mathbf{Q}_t \mathbf{u}.$$

John–Ned tracking method

- ▶ NC methods express motion in terms of WF positions A_t, B_t, \dots of **basic points or vectors** (BPVs) A, B, \dots fixed on \mathcal{R} .
- ▶ In d dimensions, d BPVs “in general position” fix \mathcal{R} uniquely.
- ▶ So in 3D we use 3 items A, B, C on \mathcal{R} .
 - ▶ A must be a point;
 - ▶ B, C can be either point or vector.



- ▶ “ $A =$ origin; B on +ve x axis; C in/toward upper xy plane.”

- ▶ Adopt **frame rule**: \mathcal{R} 's **local frame** is unique coordinates s.t.

$$[A, B, C] = \begin{bmatrix} 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & 0 \end{bmatrix} \quad \text{and the upper triangular} \\ \mathbf{R} = \begin{bmatrix} \times & \times \\ 0 & \times \end{bmatrix} \text{ has positive diagonal.}$$

- ▶ From \mathbf{R} , and whether B, C is point or vector, we precompute **constant matrix** $\mathbf{U} = \begin{bmatrix} \times & \times \\ \times & \times \\ \times & \times \end{bmatrix}$ for each body such that

$$[A_t, B_t, C_t] \mathbf{U} =: [\mathbf{i}_t, \mathbf{j}_t]$$

forms the first two vectors of \mathcal{R} 's moving ONB.

- ▶ Then cross product recovers the complete rotation matrix:

$$\mathbf{Q}_t = [\mathbf{i}_t, \mathbf{j}_t, \mathbf{i}_t \times \mathbf{j}_t].$$

To find \mathcal{R} 's KE, differentiate to get $\dot{\mathbf{Q}}_t$ and angular velocity vector $\boldsymbol{\omega}_t$, as function of $\dot{A}_t, \dot{B}_t, \dot{C}_t$. (Omit, for time reasons.)

John–Ned versus classical NCs

- ▶ **John–Ned NCs** track \mathcal{R} 's motion by 3 BPVs, storing $3 \times 3 = 9$ scalars/body, but using **nonlinear** operation $\mathbf{i}_t \times \mathbf{j}_t$.
- ▶ **Classical NCs** track by **BPVs**: $4 \times 3 = 12$ scalars/body, but **avoiding nonlinear** operation.
(In both cases fewer on average due to sharing BPVs between bodies.)
- ▶ Difference: nonlinearity gives us a **varying** mass matrix $\mathbf{M}(\mathbf{q})$, while classical NCs produce a **constant** \mathbf{M} .
Larger but constant versus smaller but varying.
 - ▶ We have more compact models.
 - ▶ DAETS handles without difficulty time varying mass matrices.

Assembly example: the RSCR

Revolute-Spherical-Cylindrical-Revolute

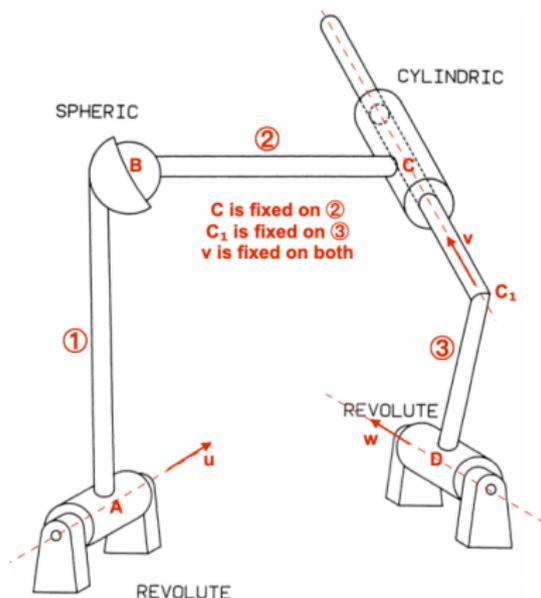
A well studied 3D mechanism with 1 DOF.

Basic points/vectors of parts:

- ① $AB\mathbf{u}$
- ② $CB\mathbf{v}$
- ③ $DC_1\mathbf{w}\mathbf{v}$

The cylindric joint is made by

- ② and ③ **sharing** \mathbf{v} .



Without loss, assume

- angles at A , C , C_1 , D are 90°
- and in WF,
- D =origin, A on $-ve$ x axis;
- w in xy plane at angle δ to x axis;
- u at angle $\langle \alpha, \beta \rangle$ in spherical polars.

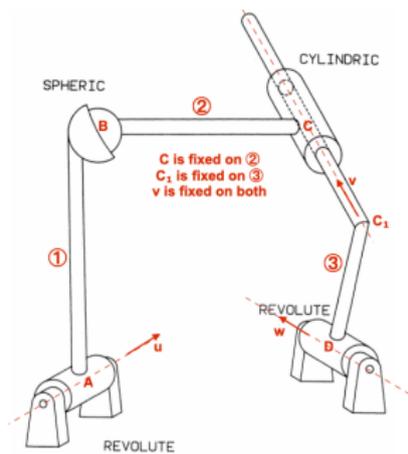
and in ③,

- v makes angle γ with w .

(Design params: 3 lengths, 4 angles.)

Take $q = (C_1, B, \mu)$, where μ is a scalar used in cylindric joint.

Total 7 scalars.



RSCR kinematics & degrees of freedom

By **assignments** we'll define vector \mathbf{v} in ③ as function of C_1 only, then share it with ② (underscore means fixed in WF):

From q	Assign	Equate	DOF
Define ③'s frame vectors, hence \mathbf{v} , and ③'s rigidity			
C_1	$\mathbf{i}_3 := C_1/L_3$	$0 = C_1^2 - L_3^2$	+3 -2
	$\mathbf{k}_3 := \mathbf{i}_3 \times \underline{\mathbf{w}}$	$0 = C_1 \cdot \underline{\mathbf{w}}$	
	$\mathbf{v} := \cos(\gamma)\underline{\mathbf{w}} + \sin(\gamma)\mathbf{k}_3$		
Define cylindric joint, and ②'s rigidity			
B, μ	$C := C_1 + \mu\mathbf{v}$	$0 = (B - C)^2 - L_2^2$	+3+1 -2
		$0 = (B - C) \cdot \mathbf{v}$	
Define ①'s rigidity			
		$0 = (B - \underline{\mathbf{A}})^2 - L_1^2$	-2
		$0 = (B - \underline{\mathbf{A}}) \cdot \underline{\mathbf{u}}$	
Net DOF:			$1 = +7 - 6$

RSCR, cont.

- ▶ To simplify dynamics let the parts be **thin uniform rigid rods** AB, BC, C₁D of masses m_1, m_2, m_3 (let joints be massless). Such a rod of mass m , moving with ends at $Y(t), Z(t)$ in WF, has KE $\frac{m}{6}(|\dot{Y}|^2 + \dot{Y} \cdot \dot{Z} + |\dot{Z}|^2)$. Then

$$\begin{aligned} T &= T_1 + T_2 + T_3 \quad (\text{Note A, D are fixed so } \dot{A} = \dot{D} = \mathbf{0}) \\ &= \frac{m_1}{6}(|\dot{B}|^2) + \frac{m_2}{6}(|\dot{B}|^2 + \dot{B} \cdot \dot{C} + |\dot{C}|^2) + \frac{m_3}{6}(|\dot{C}_1|^2) \\ &= \frac{1}{2} \dot{\mathbf{q}}^T \left(\underset{\text{const}}{\mathbf{M}_1} + \mathbf{M}_2(\mathbf{q}) + \underset{\text{const}}{\mathbf{M}_3} \right) \dot{\mathbf{q}}. \end{aligned}$$

- ▶ Dependence of \mathbf{M}_2 on \mathbf{q} is because

$$\dot{C} = \dot{C}_1 + \mu \dot{\mathbf{v}} + \dot{\mu} \mathbf{v}$$

is nonlinear in \mathbf{q} .

Compare sizes of system

- ▶ This shows length n_q of \mathbf{q} , and number n_c of constraints, in Lagrangian formulation of two examples, by classical “Jalon–Bayo” Natural Coordinates (JBNCs), and the Nedialkov–Pryce kind (NPNCs).
- ▶ Resulting DAE size is $n_q + n_c$, but $2n_q + n_c$ (in parentheses) in 1st order form for solvers such as DASSL.

	1 DOF RSCR		6 DOF robot	
	JBNCs	NPNCs	JBNCs	NPNCs
#coords n_q	13	7	30	18
#constraints n_c	12	6	24	12
DAE size	25 (38)	13	54 (84)	30

- ▶ Our savings are mainly from more economical [frames](#), and use of [assignments](#) instead of equations where possible.

Conclusion

- ▶ Modelling: write Lagrangian, constraints, etc. in Cartesian coordinates.
Much simpler than using angle coordinates and converting to an ODE.
- ▶ 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.

- ▶ **Teaching.** John & I are late to this party, but:
 - ▶ Classical NC-ers have argued for years: Cartesian coordinates make MBS ideas so easy that Lagrangian stuff can be taught at **undergraduate level**. We agree.
 - ▶ We can add: with DAETS the DAEs are now as easy as ODEs.
- ▶ Our infrastructure should be good at **important tasks** such as:
 - ▶ Finding stationary equilibrium configuration.
 - ▶ Inverse dynamics: torques etc. that give a desired motion.
 - ▶ Kinematic design, e.g. make RSCR move optimally near a desired curve.

References

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- ▶ JP, NN, G. Tan, X. Li (2018) How AD can help solve differential-algebraic equations
Optimization Methods and Software, 33:4-6, 729-749
- ▶ B. Derakhshan. Multibody Dynamics Problems in Natural Coordinates: Theory, Implementation and Simulation
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▶ YouTube Multi-body Lagrangian Simulations

- ▶ Outer planets

- ▶ Gravitating masses in 2D

- ▶ Rods, plate, springs, particles, collinears

- ▶ RSCR Chebyshev linkage version

- ⋮

Example: Mechanism0

- ▶ Rod **OA** pivots at fixed point **O**.
- ▶ Spring **AB** attached at **A**.
- ▶ Particle attached at **B**.
- ▶ System moves under gravity.
- ▶ [Animation](#)

Mechanism0: specification in YAML

Title: Mechanism0

Dimension: 2

PhysicalParams:

{ L: 1, M: 1, k: 500, l: 1, mu: .5, m: 2 }

PartData:

Fixed: { O: [0, 0] }

Rigids:

OA:

Geom: [[L, 0]] # local frame geometry
centroid, mass, moment of inertia

Dyna: [[L/2, 0], M, M*L**2/12]

Springs:

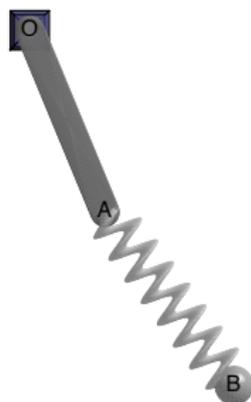
AB: [k, l, mu] # stiffness, length, mass

Particles :

B: m # mass

AppliedForces:

Gravity: #turns it on with default value

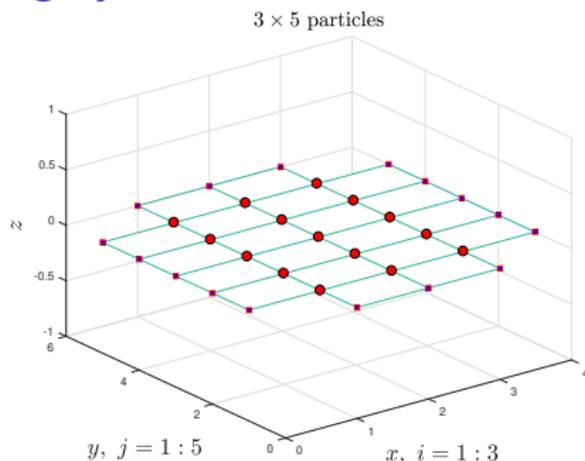


Mechanism0: IVs; solver & animation settings

```
ProblemData: # integration interval, etc.  
  t0: 0  
  tend: 20  
  positions: { A: [L, 0], B: [(L+1), 0] } # guesses for A, B  
  fixedpositions: { Ax, B } # don't change values for A.x, B  
  velocities: { Ay: 10, B: [0, 0] }  
SolverParams: # to guide DAETS  
  Integration:  
    tol: 1e-12  
    order: 20  
Animation: # to guide animation  
  Scene:  
    view: [0, 90] # camera azimuth, elevation
```

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 $\mathbf{r}_{ij} = (x_{ij}, y_{ij}, z_{ij})$ full 3D motion
 - ▶ mass M
- ▶ Each spring
 - ▶ stiffness k
 - ▶ length at rest l
 - ▶ damping $k_d \times$ stretch-rate (except the boundary ones)
- ▶ Spacing Δx and Δy between particles in x and y directions.
- ▶ Initially all particles at rest in xy plane, we push the middle particle upwards.
- ▶ ▶ Animation 90×90 particles, 24,300 second-order ODEs.

Particle-spring cont

- ▶ Energy contributions

	KE	PE
Particle (i, j)	$\frac{1}{2}M \dot{\mathbf{r}}_{ij} ^2$	Mgz_{ij}
Spring $(i, j)-(i, j+1)$		$\frac{1}{2}(\mathbf{r}_{i,j+1} - \mathbf{r}_{ij} - l)^2$

Add up over whole mesh to get T , V and then $\mathcal{L} = T - V$.

- ▶ Spring $(i, j)-(i, j+1)$ dissipation

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

Add up to obtain Rayleigh dissipation function R .

- ▶ Lagrangian facility takes \mathcal{L} and R and produces 2nd-order ODE of size $3mn$

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}_{ij}} - \frac{\partial \mathcal{L}}{\partial \mathbf{r}_{ij}} + \frac{\partial R}{\partial \dot{\mathbf{r}}_{ij}} = 0, \quad i = 1 : m, \quad j = 1 : n$$

which DAETS integrates.