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Data-Driven Mechanics: Constitutive Model-Free Approach

$$\inf_{y\in D}\inf_{z\in E}\|y-z\| = \inf_{z\in E}\inf_{y\in D}\|y-z\|$$

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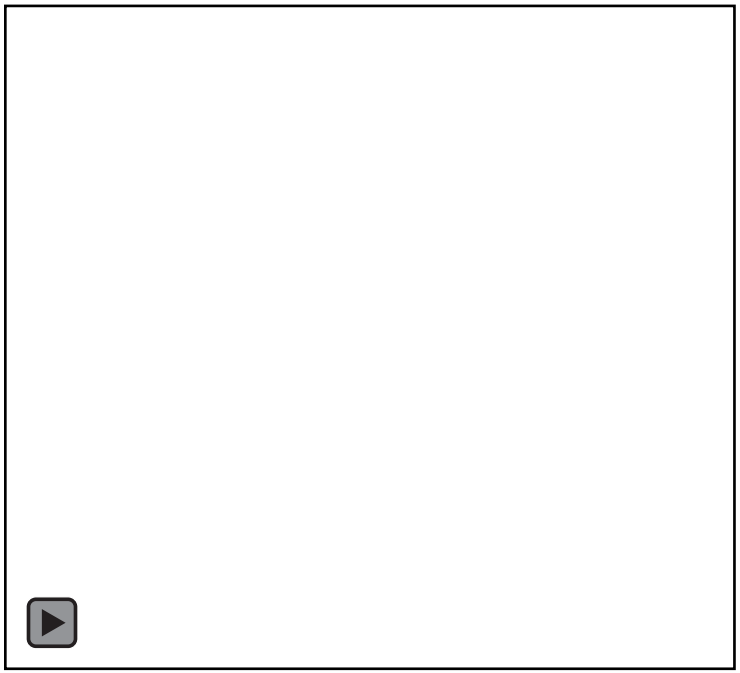
California Institute of Technology and
Rheinische Friedrich-Wilhelms Universität Bonn

Centre International des Sciences Mécaniques (CSIM)
Udine (Italy), October 10-14, 2022

Structural/solid dynamics



- Phase space: $Z = \mathbb{R}^N \times \mathbb{R}^N$.
- To determine: Trajectories $z(\cdot)$ over $[0, T]$.
- Space of trial trajectories:

$$\mathcal{Z} \equiv \{z(\cdot) = (\epsilon(\cdot), \sigma(\cdot)) : [0, T] \to Z\}.$$

- NB: $z(t) =$ value of $z(\cdot)$ at $t \in [0, T]$.
- Space of physically admissible trajectories,

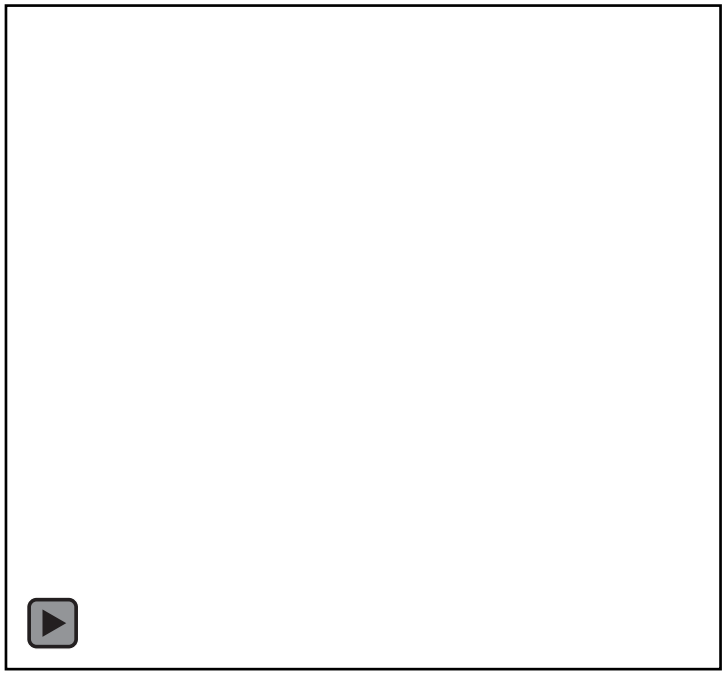
$$\mathcal{E} = \Big\{ z(\cdot) \equiv (\epsilon(\cdot), \sigma(\cdot)) \in \mathcal{Z} \ : \ \text{for } t \in [0, T],\ \epsilon_e(t) = B_e u(t),$$
$$M\ddot{u}(t) + \textstyle\sum_{e=1}^{m} w_e B_e^T \sigma_e(t) = f(t); \quad u(0) = u_0,\ \dot{u}(0) = v_0 \Big\}.$$

- Space of material trajectories: For given material set D,

$$\mathcal{D} = \big\{ y(\cdot) = (\epsilon(\cdot), \sigma(\cdot)) \in \mathcal{Z} \ : \ (\epsilon(t), \sigma(t)) \in D,\ t \in [0, T] \big\}.$$

- Classical phase-space trajectories: $z(\cdot) \in \mathcal{D} \cap \mathcal{E}$,
  - Admissible trajectories that are material!
  - Material trajectories that are admissible!

Structural/solid dynamics



- D may consist of empirical point data.
- No classical trajectories! $(\mathcal{D} \cap \mathcal{E} = \emptyset)$.
- Need Data-Driven reformulation!
- Metrize space $\mathcal{Z}$ of trajectories, e. g.,

$$\|z(\cdot)\| = \left(\int_0^T \|z(t)\|^2 \, dt \right)^{1/2}.$$

- Data-Driven trajectories:

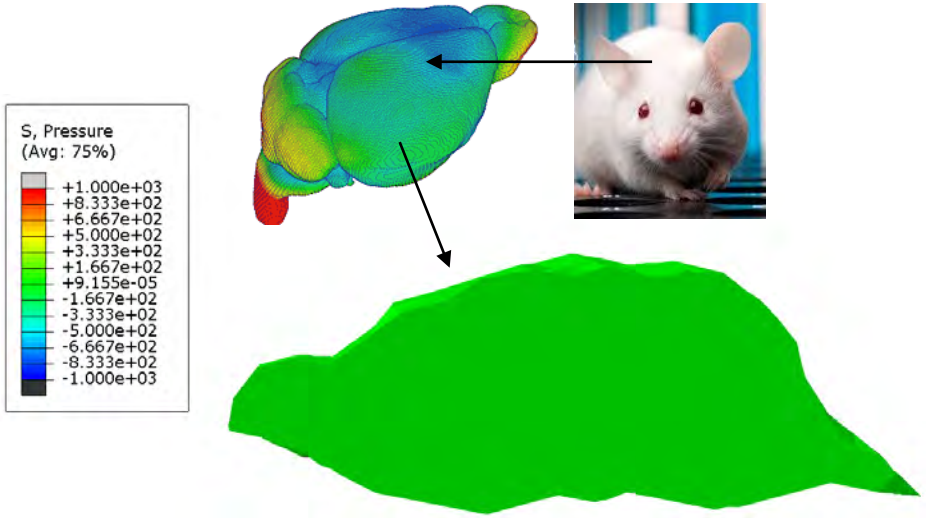
$$\big(y(\cdot), z(\cdot)\big) \in \operatorname{argmin}\Big\{ \|y(\cdot) - z(\cdot)\|^2 \, : \, y(\cdot) \in \mathcal{D}, \; z(\cdot) \in \mathcal{E} \Big\},$$

  - Admissible trajectories that are closest to being material.
  - Material trajectories that are closest to being admissible.

- Implementation: With $y(\cdot) \in \mathcal{D}$, $z(\cdot) = (\epsilon(\cdot), \sigma(\cdot)) \in \mathcal{Z}$,
  - Enforce compatibility strongly by setting $\epsilon_e(t) = B_e u(t)$.
  - Enforce dynamic equilibrium by means of Lagrange multiplier $w(\cdot)$,

$$\delta\Big\{ \int_0^T \|y(t) - z(t)\|^2 \, dt + \int_0^T \Big(M\ddot{u}(t) + \sum_{e=1}^m w_e B_e^T \sigma_e(t) - f(t) \Big) \cdot w(t) \, dt \Big\} = 0 \, .$$

Structural/solid dynamics



- Time discretization:
  $t_0, \ldots, t_k, t_{k+1} = t_k + \tau, \ldots, t_N.$
- Space of discrete trial trajectories:
  $$\mathcal{Z}_\tau \equiv \{z_\cdot = (\epsilon_\cdot, \sigma_\cdot) : [0, \ldots, N] \to Z\}.$$
- NB: $z_k =$ value of $z_\cdot$ at $k \in [0, \ldots, N]$.
- Space of physically admissible discrete trajectories,
  $$\mathcal{E}_\tau = \Big\{ z_\cdot \equiv (\epsilon_\cdot, \sigma_\cdot) \in \mathcal{Z}_\tau \ : \text{for } k \in [0, \ldots, N],\ \epsilon_{e,k} = B_e u_k,$$
  $$M \frac{u_{k+1} - 2u_k + u_{k-1}}{\tau^2} + \sum_{j=-n}^{n} \alpha_j \Big(\sum_{e=1}^{m} w_e B_e^T \sigma_{e,k+j} - f_{k+j} \Big) = 0 \Big\}.$$
- Space of material trajectories: For given material set D,
  $$\mathcal{D}_\tau = \big\{ y_\cdot = (\epsilon_\cdot, \sigma_\cdot) \in \mathcal{Z}_\tau \ : \ (\epsilon_k, \sigma_k) \in D,\ k \in [0, \ldots, N] \big\}.$$
- Discrete Data-Driven trajectories: With metric $\|y_\cdot - z_\cdot\|^2 = \sum_{k=0}^{N} \|y_k - z_k\|^2 \tau$,
  $$\big(y_\cdot, z_\cdot\big) \in \operatorname{argmin} \Big\{ \|y_\cdot - z_\cdot\|^2 \ : \ y_\cdot \in \mathcal{D},\ z_\cdot \in \mathcal{E} \Big\},$$
  - Admissible discrete trajectories that are closest to being material.
  - Material discrete trajectories that are closest to being admissible.

Structural/solid dynamics

- Equivalent Newmark parameters:

$$\alpha_{-1} = \frac{1}{2} + \beta - \gamma, \quad \alpha_0 = \frac{1}{2} - 2\beta + \gamma, \quad \alpha_1 = \beta.$$

- Explicit dynamics: $\beta = 0$, $\gamma = 1/2$.
- Central differences, Verlet: $\alpha_{-1} = \alpha_1 = 0$, $\alpha_0 = 1$.

C60 fullerene

Algorithm Explicit Data-Driven dynamics

Require: Time step τ; arrays u_{k-1}, u_k, σ_k and f_k; material data set D. Then:

i) Compute u_{k+1} from:

$$M\frac{u_{k+1} - 2u_k + u_{k-1}}{\tau^2} + \sum_{e=1}^{m} w_e B_e^T \sigma_{e,k} = f_k.$$

ii) Update strains: Set $\epsilon_{e,k+1} = B_e u_{k+1}$.

iii) Find $(\alpha_{k+1}, \beta_{k+1})$ in D such that α_{k+1} is closest to ϵ_{k+1}.

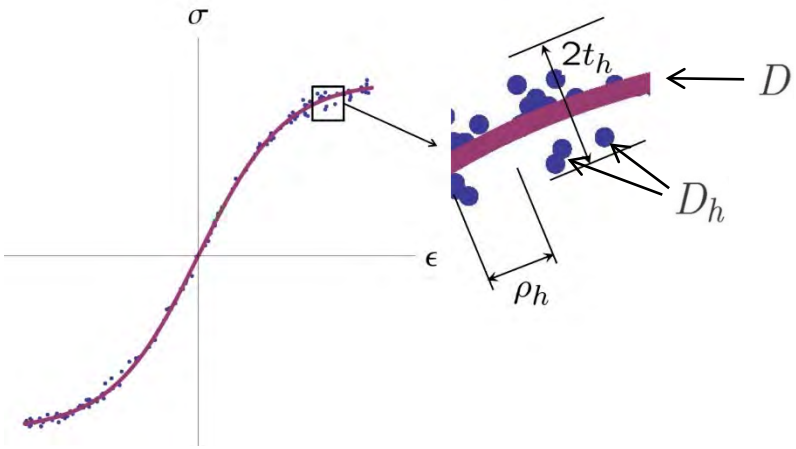
iv) Update stresses: Set $\sigma_{k_+1} = \beta_{k_+1}$.

Return u_n, u_{k+1} and f_{k+1}.

Convergence with respect to the data

- Initial-value problem:

$$M\ddot{u}(t) + \sum_{e=1}^{m} w_e B_e^T \hat{\sigma}_e(B_e u(t)) = f(t),$$
$$u(0) = u_0, \quad \dot{u}(0) = v_0.$$



Theorem (Uniform convergence)

Let (D_h) be a sequence of local material data sets generated by sampling exact material laws $\hat{\sigma}_e$ with observational error. Assume:

i) *(Non-degenerate mass) $M > 0$,there is $m > 0$ s. t. $\|M\| \geq m$, $\|M^{-1}\| \leq m^{-1}$.*

ii) *(Lipschitz materials) $\hat{\sigma}_e : \mathbb{R}^d \to \mathbb{R}^d$ Lipshitz, $u(\cdot) \in W^{1,\infty}([0,T],\mathbb{R}^n)$ unique.*

iii) *(Uniform sampling) There is $\delta_h \downarrow 0$ s. t., $\forall z \in Z$, $\exists\, y \in D_h$ with $\|y - z\| \leq \delta_h$.*

Then, the Data-Driven solutions $u_h(\cdot) \to u(\cdot)$ strongly in $W^{1,\infty}((0,T),\mathbb{R}^n)$.

- Recall (R. Abraham, J. E. Marsden and T. Ratiu, "Manifolds, Tensor Analysis, and Applications", Springer-Verlag, New York, NY, 3rd edition, 2001):
  - Lemma 4.1.6: if $\hat{\sigma}$ Lipschitz, there is unique C^1 solution over some $[0,T]$.
  - Example 4.1.23B: If $(1/m)V(q) \geq a - b\|q\|^2$, $b \geq 0$, solutions exist for all time.

Convergence with respect to the data

Proof sketch. *(assigned reading, refer to notes for full proof)*

- Estimating the Euler-Lagrange equations using uniform sampling assumption (iii),

$$\|w_h(t)\| \leq \frac{CT^2}{m}\delta_h \Rightarrow w_h(t) \to 0 \text{ uniformly in } [0,T].$$

- Subtracting equations of motion, integrating and estimating,

$$m\|\dot{u}_h(t) - \dot{u}(t)\| \leq \int_0^t C\|\beta_h(t') - \hat{\sigma}(Bu(t'))\|\, dt' + \frac{CT^3}{m}\delta_h.$$

- By Lipschitz continuity (ii) and the uniform sampling assumption (iii),

$$\|\beta_h(t) - \hat{\sigma}(\epsilon(t))\| \leq (1+L)\delta_h + L\,\|\epsilon_h(t) - \epsilon(t)\|.$$

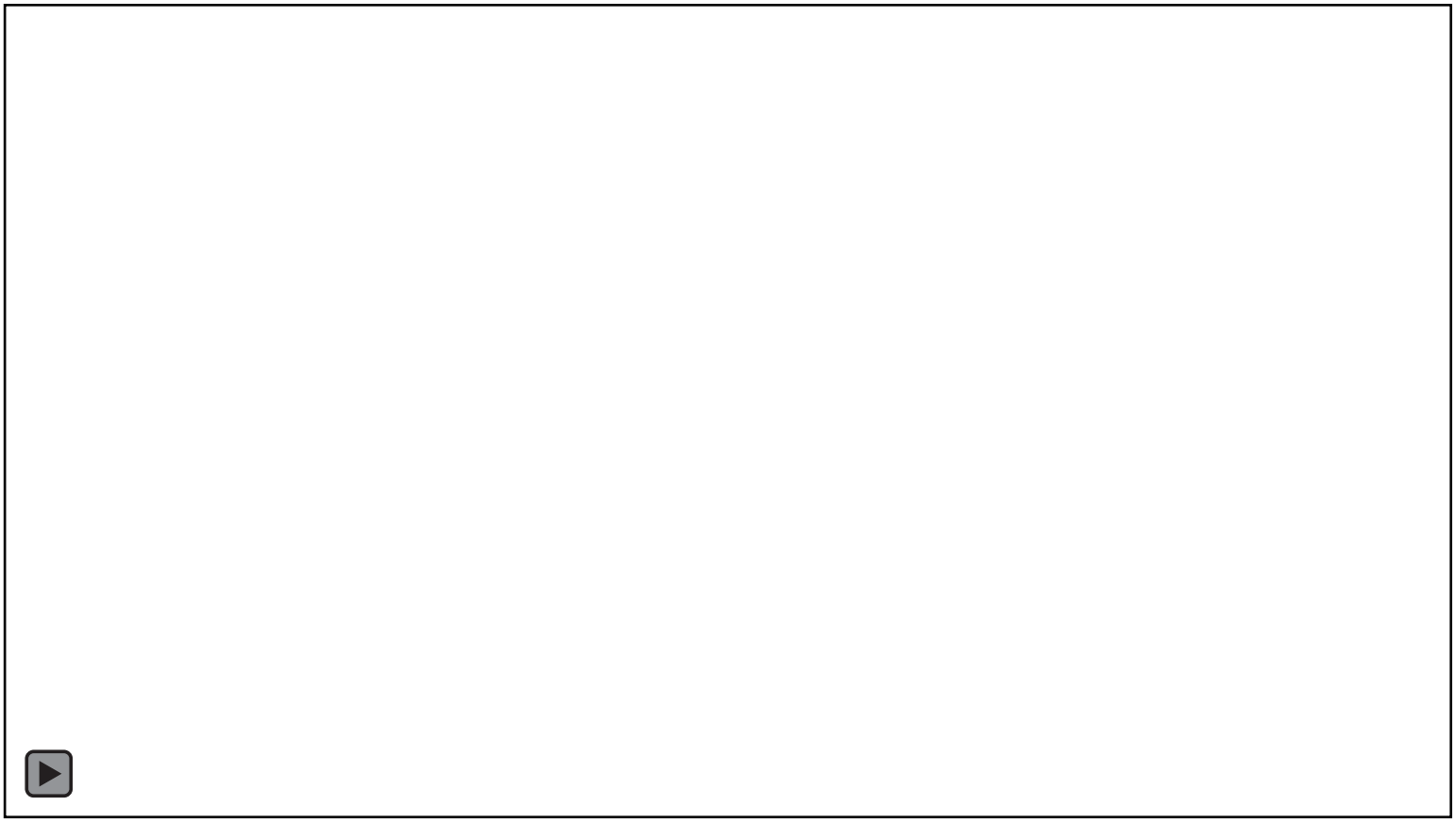
- By Pointcaré's inequality,

$$m\|\dot{u}_h(t) - \dot{u}(t)\| \leq C'L\frac{T}{\pi}\int_0^t \|\dot{u}_h(t') - \dot{u}(t')\|\, dt' + C\left((1+L)T + \frac{T^3}{m}\right)\delta_h.$$

- By Gronwall's inequality,

$$\|\dot{u}_h(t) - \dot{u}(t)\| \leq \left[1 + \frac{TC'L}{\pi m}t\exp\left(\frac{TC'L}{\pi m}t\right)\right]\left(\frac{LT}{m} + \frac{CT^3}{m^2}\right)\delta_h.$$ ∎

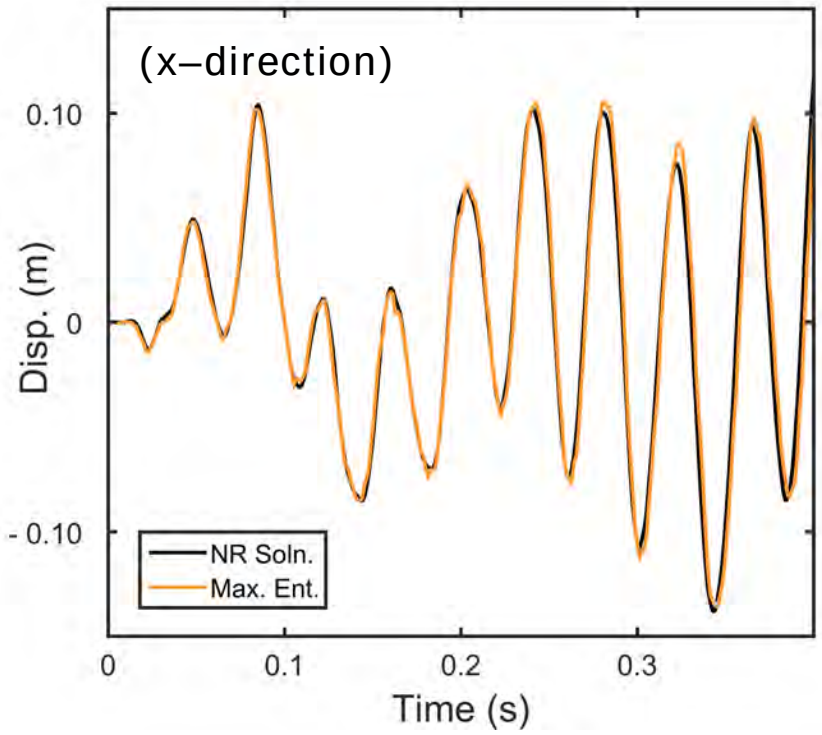
Convergence with respect to the data

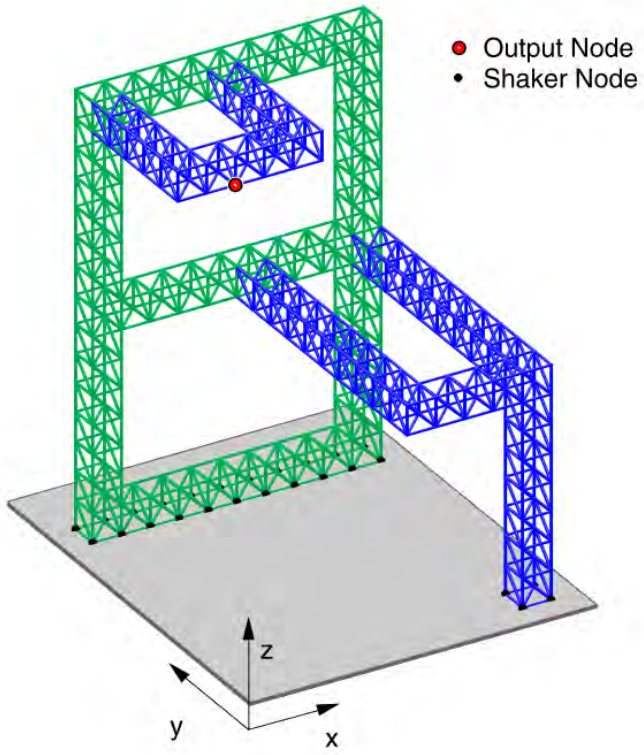


3D truss structure shaking under ground motion.
Random data sets generated according to capped
normal distribution centered on the true material curve
Data-Driven dynamics solution and data coverage

T. Kirchdoerfer and M. Ortiz, *IJNME*, **113**(11) (2018) 1697-1710.

Convergence with respect to the data

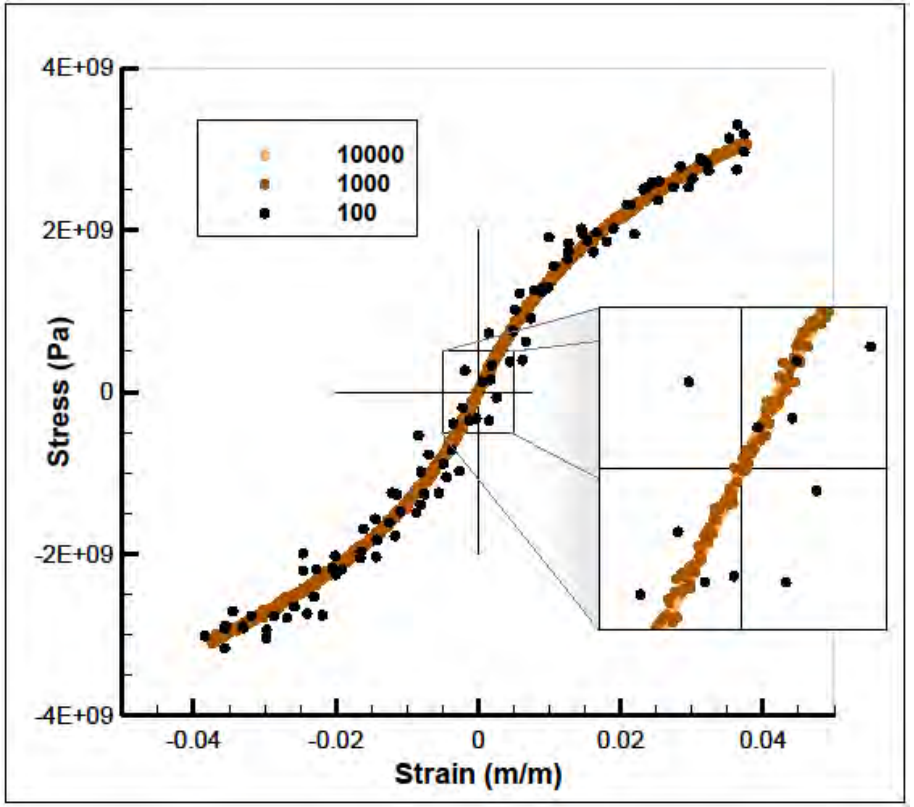


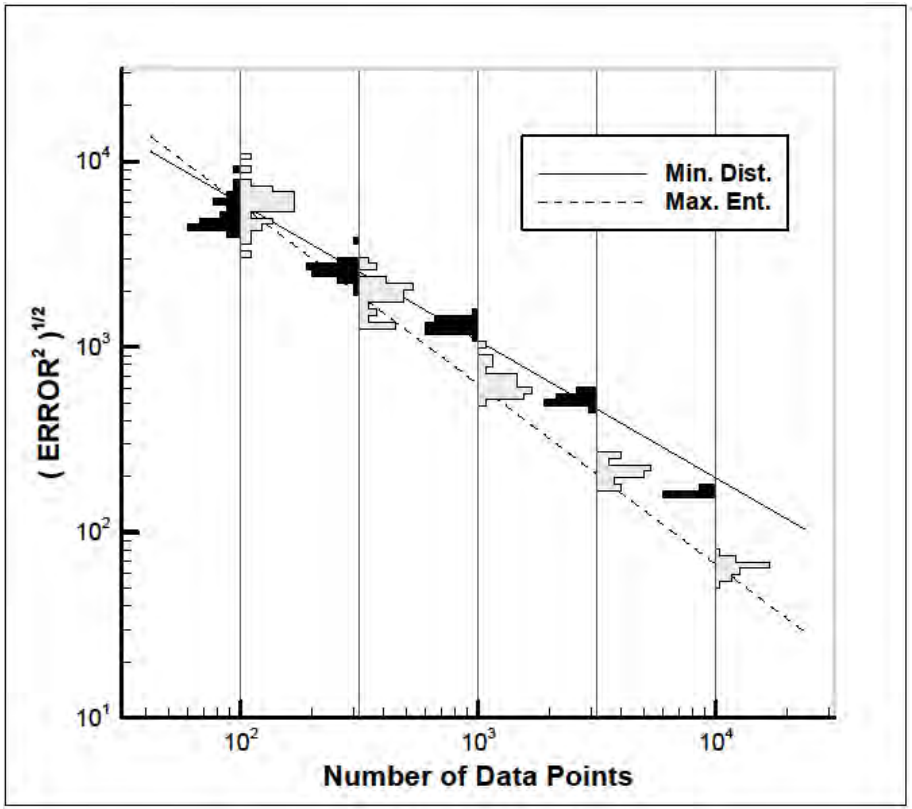


3D truss structure shaking under ground motion.
Random data sets generated according to capped normal distribution centered on the true material curve
Data-Driven solution vs direct Newmark solution

T. Kirchdoerfer and M. Ortiz, *IJNME*, **113**(11) (2018) 1697-1710.

Convergence with respect to the data





3D truss structure shaking under ground motion.
Random data sets generated according to capped normal distribution
centered on the true material curve with standard deviation
in inverse proportion to the square root of the data set size

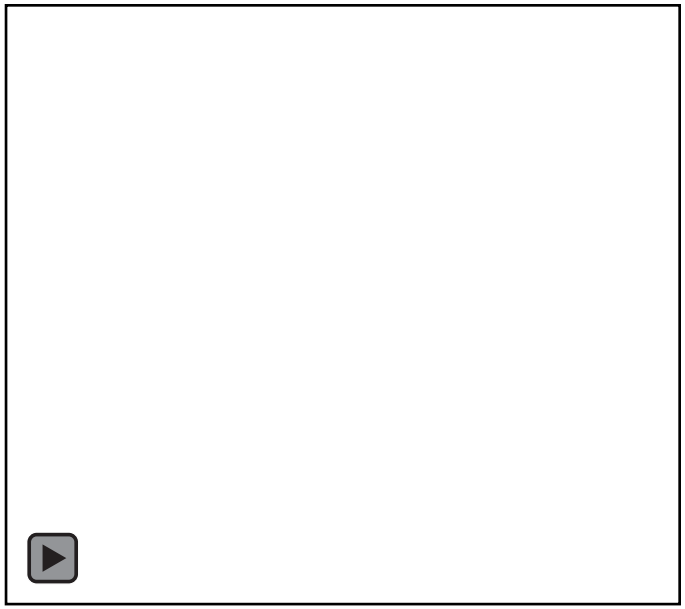
T. Kirchdoerfer and M. Ortiz, *IJNME*, **113**(11) (2018) 1697-1710.

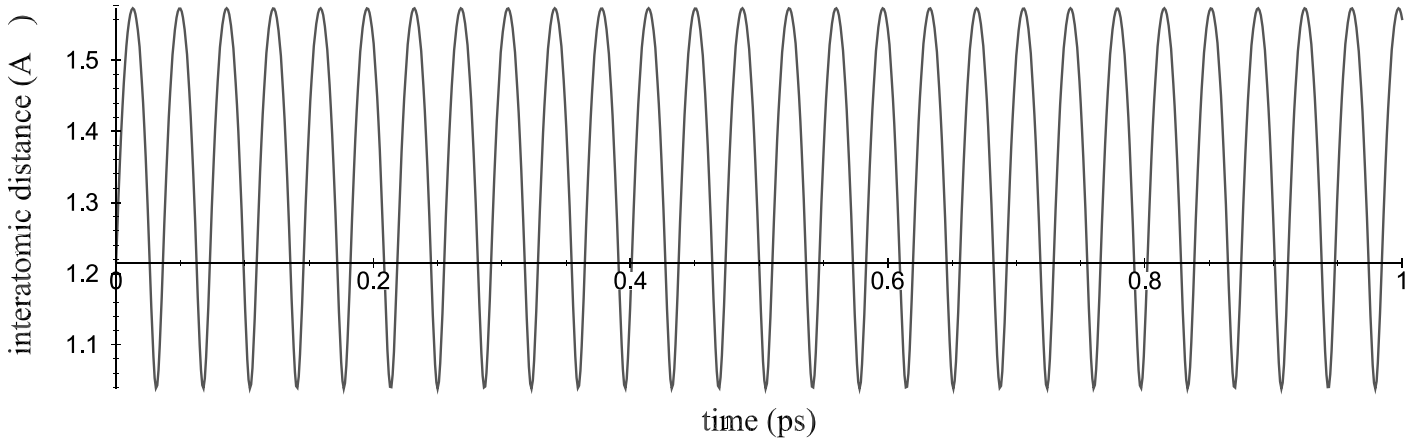
Convergence with respect to the data

- Molecular oxygen O_2.
- Morse potential:

$$V(r) = D_e\left(\mathrm{e}^{2a(r_e-r)} - 2\mathrm{e}^{a(r_e-r)}\right)$$

- Parameters fitted to diatomic constants in: K. P. Huber and G. H. Herzberg, NIST Chemistry WebBook.

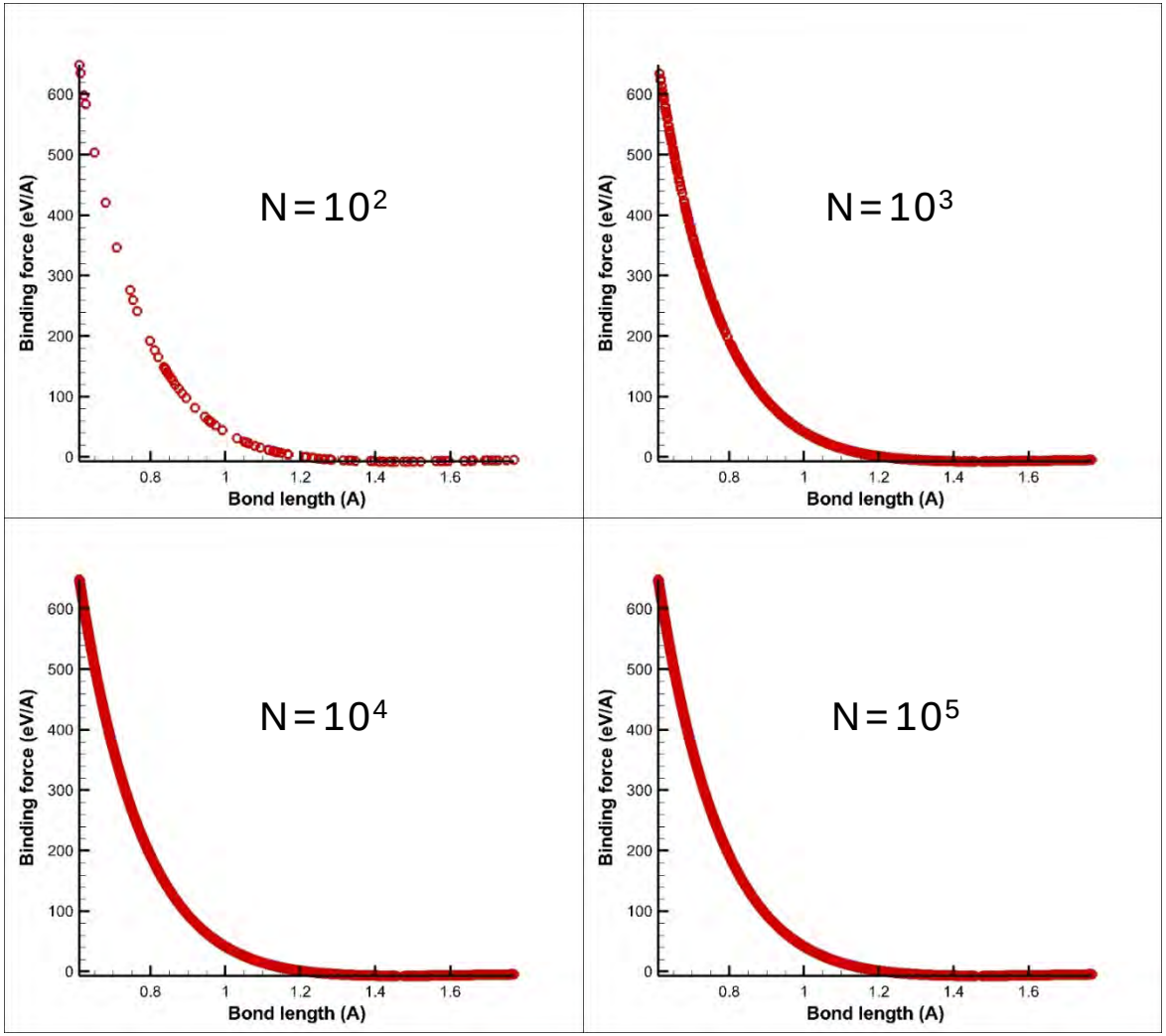




Bulin, J., Hamaeckers, J., Ariza, P. and Ortiz, M., arXiv:2208.04937

Convergence with respect to the data

- Sampling of Morse force field $\Rightarrow$ data sets D.

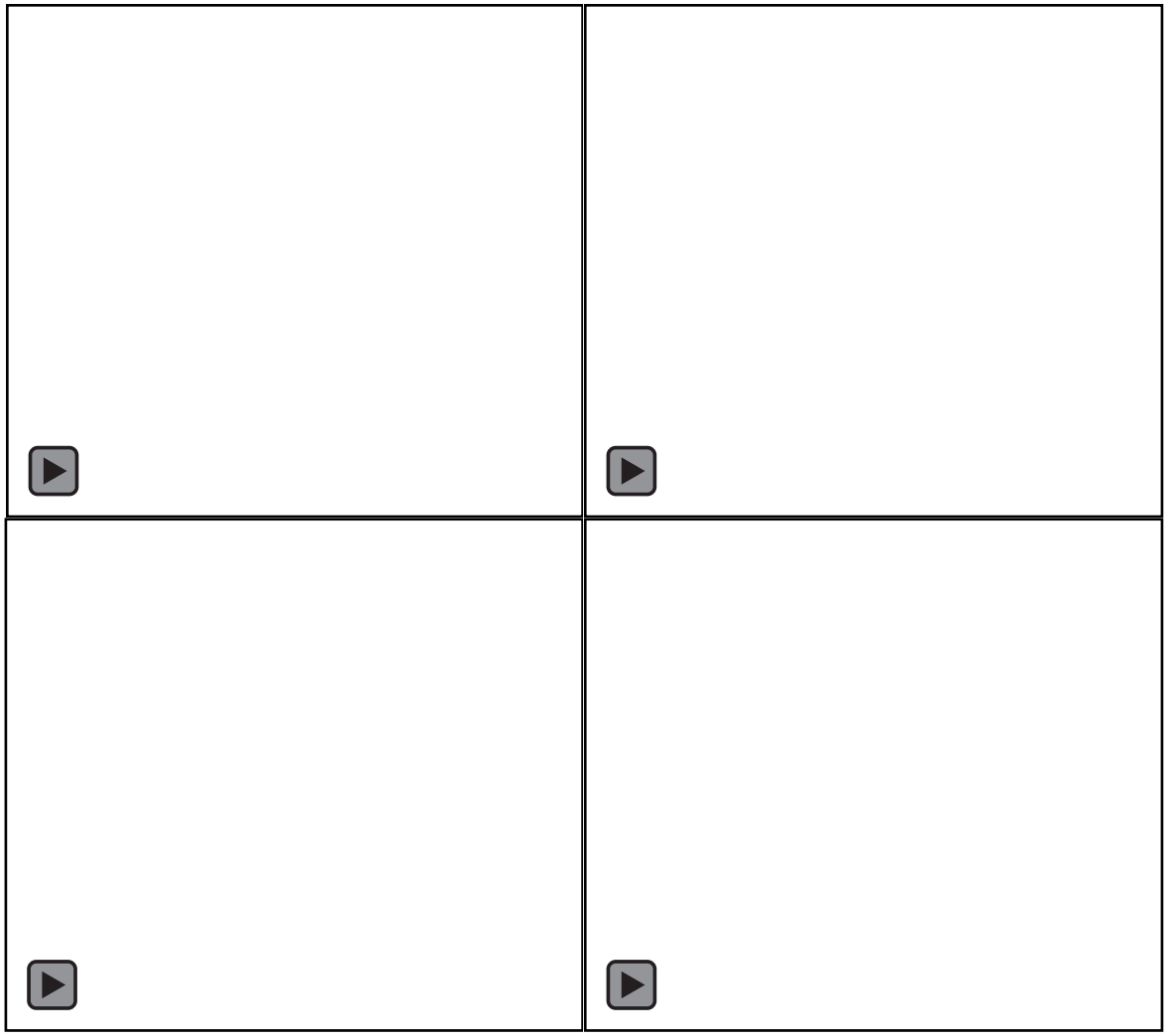


Bulin, J., Hamaeckers, J., Ariza, P. and Ortiz, M., arXiv:2208.04937

Convergence with respect to the data

- Data-Driven Verlet trajectories computed from data sets of increasing size.

$N = 10^2$ $N = 10^3$

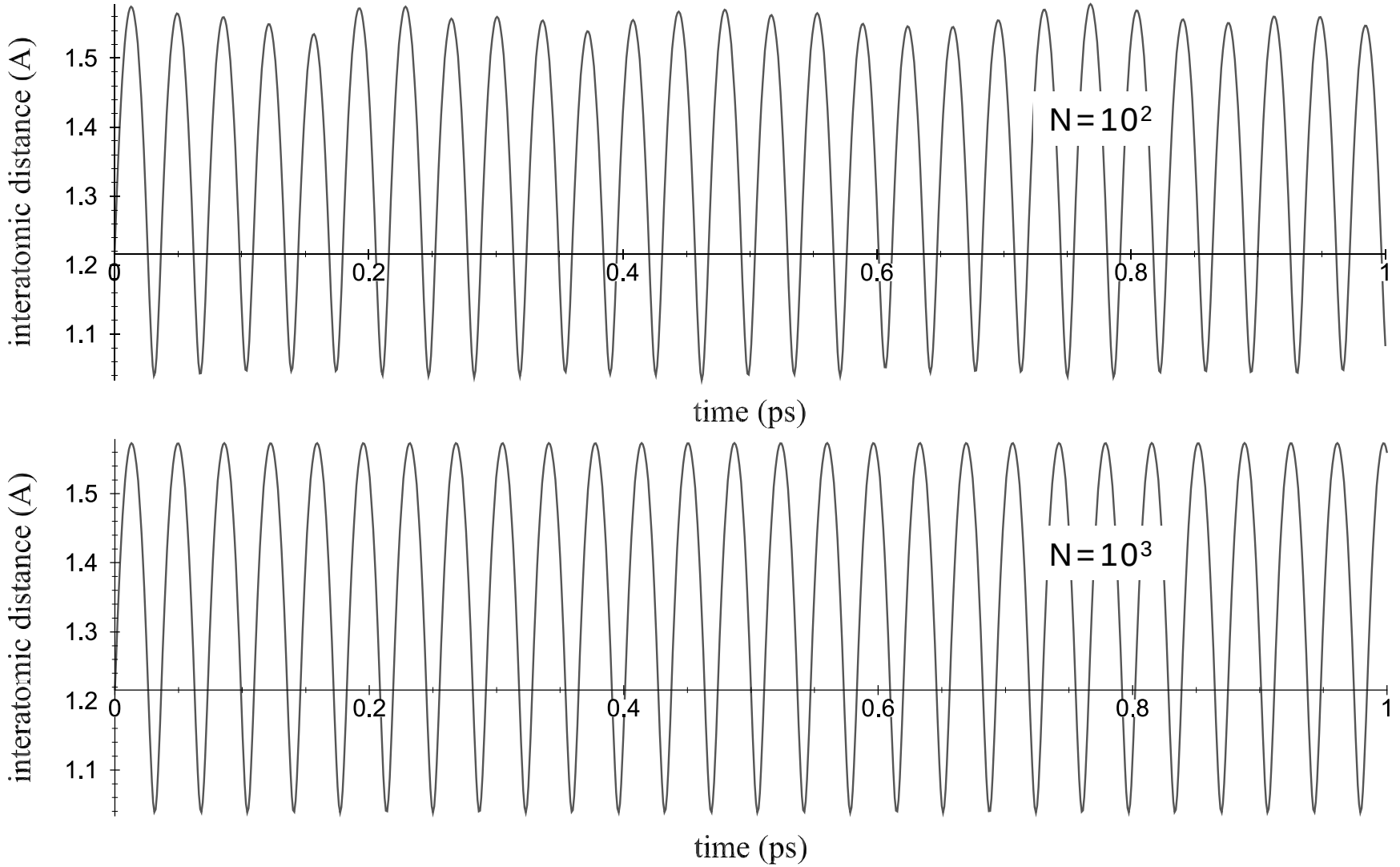


$N = 10^4$ $N = 10^5$

Bulin, J., Hamaeckers, J., Ariza, P. and Ortiz, M., arXiv:2208.04937

Convergence with respect to the data

- Data-Driven Verlet trajectories computed from data sets of increasing size.



Bulin, J., Hamaeckers, J., Ariza, P. and Ortiz, M., arXiv:2208.04937

Convergence with respect to the data

- Molecular oxygen O_2.
- Error norm:

$$\|u\| = \left(\int_0^{+\infty} |u(t)|^2 \, \frac{dt}{t^2} \right)^{1/2}$$

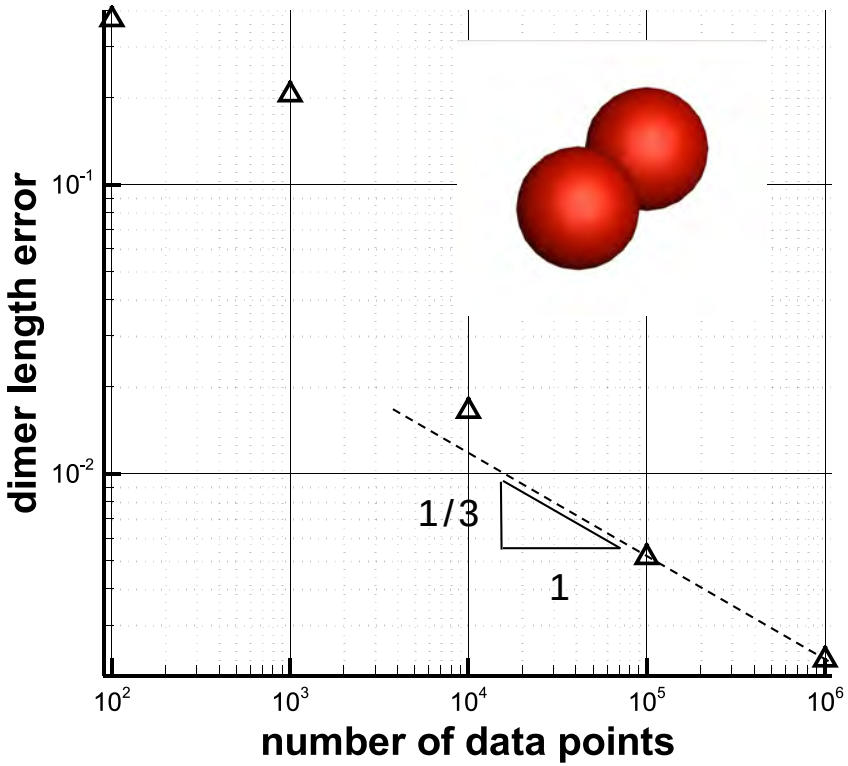
- Amplitude error:

$$\|A' \sin \omega t - A'' \sin \omega t\| = \sqrt{\frac{\pi\omega}{2}} |A' - A''|$$

- Frequency error:

$$\|A \sin \omega' t - A \sin \omega'' t\| = \sqrt{\frac{\pi}{2}} |A| \, |\omega' - \omega''|$$

- Data-Driven Verlet trajectories converge to exact Morse trajectory in amplitude and in frequency with increasing data-set size.

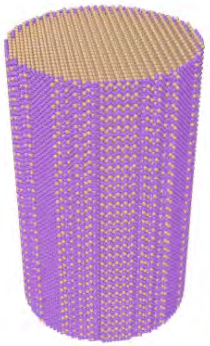


Convergence plot, Data-Driven Verlet *vs.* exact Morse solution

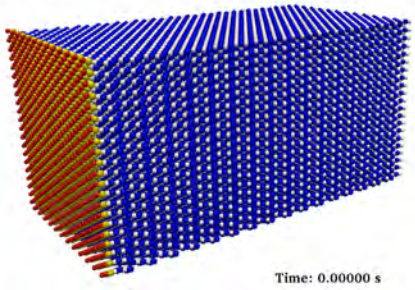
Bulin, J., Hamaeckers, J., Ariza, P. and Ortiz, M., arXiv:2208.04937

Interatomic-potential-free Data-Driven molecular dynamics

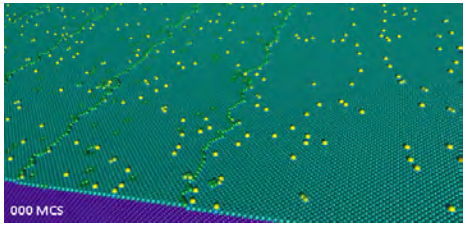
- Field of application: Molecular dynamics, computational materials science.



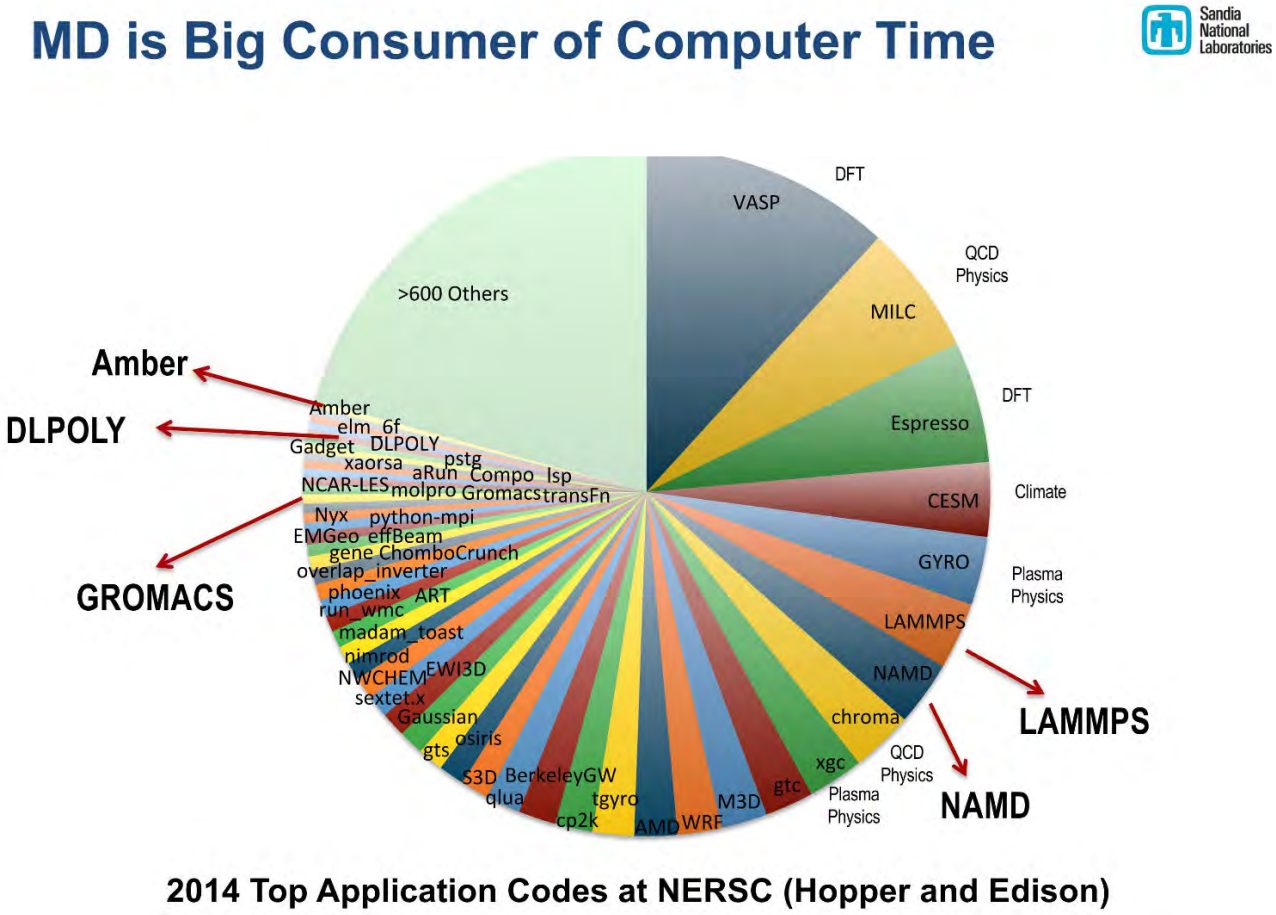
Silicon lithiation[1]



Palladium hydration[2]



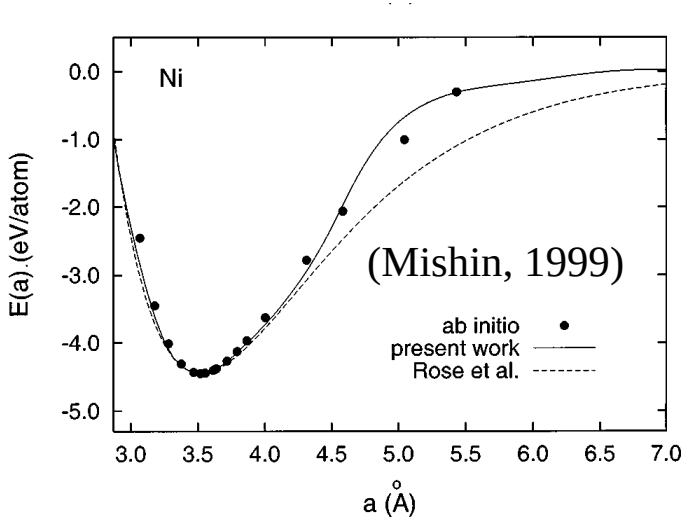
Surface diffusion[3]



[1]J.P. Mendez, M. Ponga, M. Ortiz, *JMPS*, **115** (2018) 123-141.
[2]K.G. Wang, M. Ortiz, M.P. Ariza, *Int. J. Hydrog. Energy*, **40**(15) (2015) 5353-5358.
[3]Courtesy of: Dr. Lars Röntzsch, Dresden, Germany

Interatomic-potential-free Data-Driven molecular dynamics

- Governing equation: $F = ma$ (Sir Isaac Newton, 1687).
- Elementary, except for:
  - $a = \ddot{r} \in \mathbb{R}^N$, $N \sim 6.022 \times 10^{23}$/mol (A. Avogadro, 1811).
  - Thermal vibrations on femtosecond scale $\ll$ macroscale.
  - Force system F is unknown!
- Conservative systems:
  - Interatomic potential: $V(r)$.
  - Force field: $F(r) = DV(r)$.
- Standard practice:
  - Parameterized potentials.
  - Nonlinear regression.
  - *ab initio* training sets.

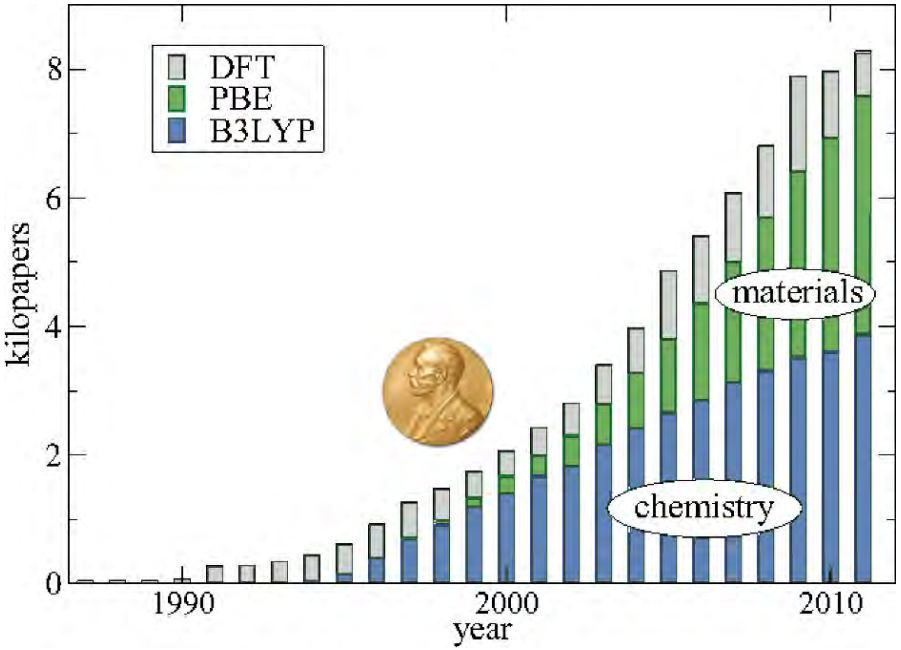


- No guarantees of accuracy, stability, convergence.

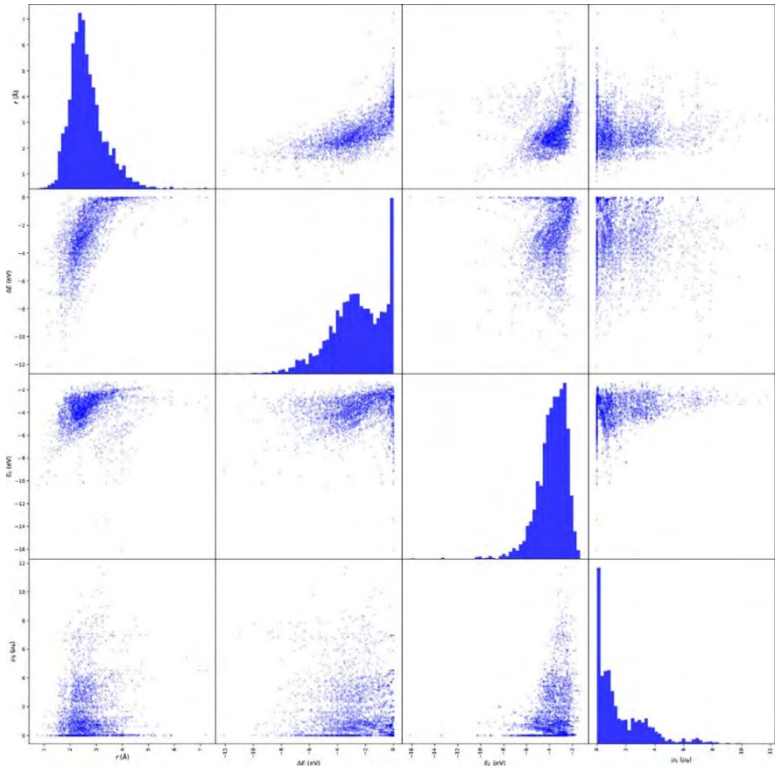
Y. Mishin *et al.*, *Phys. Rev. B*, **59** (1999) 3393-3407.

Interatomic-potential-free Data-Driven molecular dynamics

- Unprecedented *availability of accurate material data* from *ab initio* atomistic calculations (QM, DFT): New challenges and opportunities for Data Science



Numbers of DFT papers per year (source: Web of Knowledge).[1]



3916 *diatomic systems* and 88 isolated atom systems evaluated using VASP: *interatomic distance, binding energy*, Fermi energy and spin magnetic moment.[2]

[1]K. Burke, *J. Chem. Phys.*, **136** (2012) 150901.
[2]K. Shibata, E. Suzuki, T. Mizoguchi, *Data in Brief*, **36** (2021) 106968.

Interatomic-potential-free Data-Driven molecular dynamics

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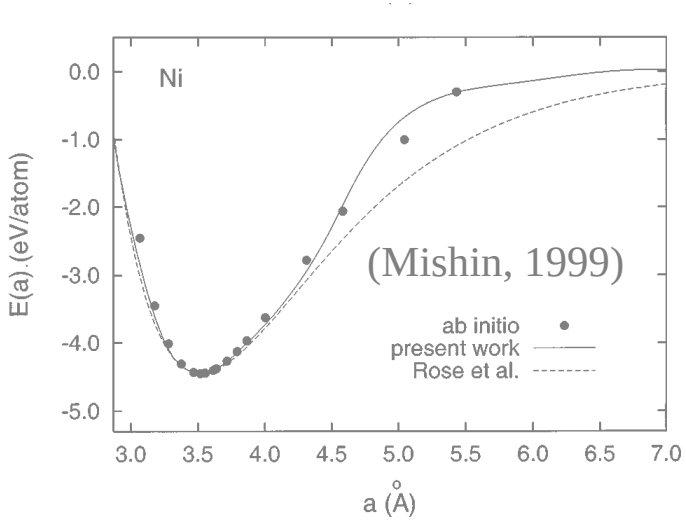
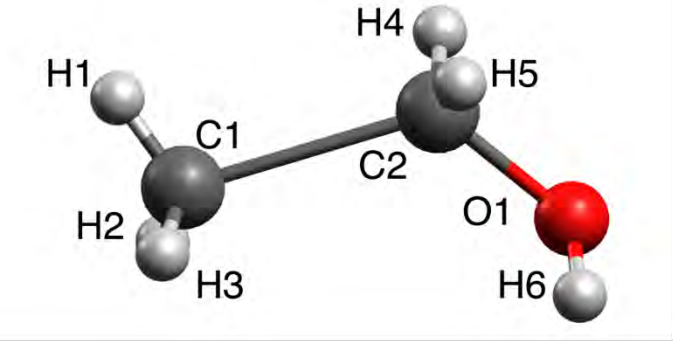


- No guarantees of accuracy, stability, convergence.
- Instead: Use data sets directly in calculations!

Y. Mishin *et al.*, *Phys. Rev. B*, **59** (1999) 3393-3407.

Interatomic-potential-free Data-Driven molecular dynamics

- Properties of force fields:
  - Locality (short range of interaction).
  - Invariance under Euclidian group $E(3)$ of isometries in Euclidean space $\mathbb{E}^3$: Translations, rotations, reflections.



- Consequences of locality:
  - For $i = 1, \ldots, n \equiv$ number of atoms,

$$f_i(r) = f_i(r_i; \{r_j \ : \ j \in N_i\}) = \frac{\partial V_i}{\partial r_i}(r_i; \{r_j \ : \ j \in N_i\}).$$

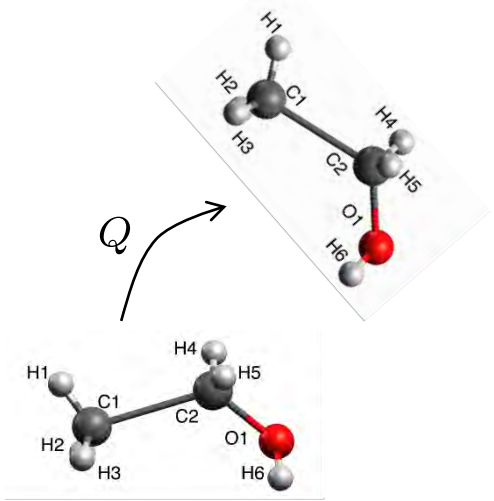
  - $N_i :=$ local neighborhood of atom i (e. g., $\{|r_j - r_i| \leq r_c\}$).

- Consequences of $E(3)$-invariance:
  - Invariance under translations:

$$\text{Strain: } \epsilon_i \equiv \{r_{ij} = r_j - r_i \ : \ j \in N_i\} \equiv B_i r,$$
$$\text{Stress: } \sigma_i \equiv \{f_{ij} \ : \ j \in N_i\} = \hat{\sigma}_i(\epsilon_i) = DV_i(\epsilon_i),$$
$$\text{Eqs. of motion: } M\ddot{r} + \Sigma_{i=1}^n B_i^T \sigma_i = f^{\text{ext}}(t).$$

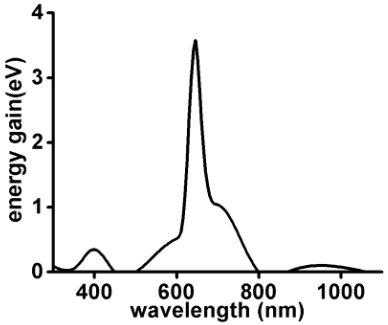
  - Invariance under $O(3)$ (rotations+reflections):

$$\sigma_i = \hat{\sigma}_i(\epsilon_i) \Leftrightarrow Q\sigma_i = \hat{\sigma}_i(\epsilon_i), \quad \forall Q \in O(3).$$



Interatomic-potential-free Data-Driven molecular dynamics

- Test case: Radiation-induced fragmentation of C60 fullerene.
- In intense laser field, the breathing vibrational mode is strongly excited.
- The extent of energy deposition depends on radiation frequency, is maximum at wavelength $\sim$ 700 nm.
- C60 fullerene is a common model for studying the mechanisms of molecular energy deposition and migration in intense laser field.



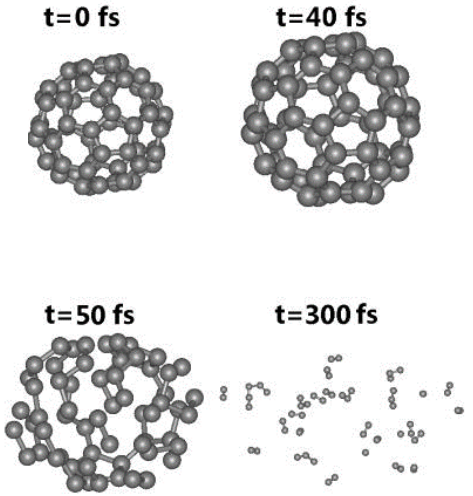
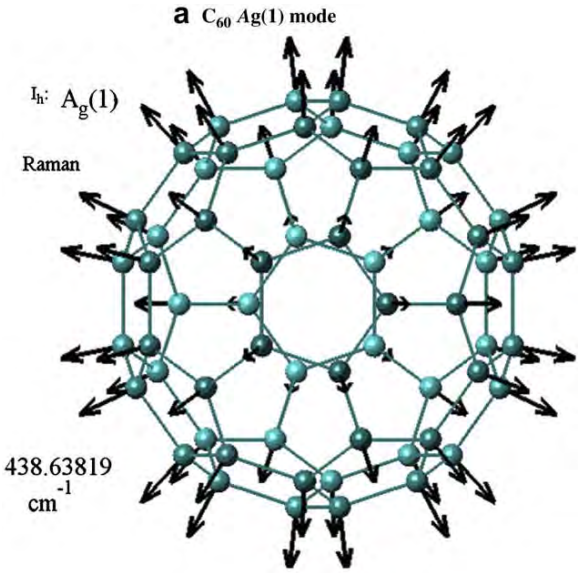


Table 1
Calculated and experimental Raman vibrational frequencies for C_{60} (cm^{-1}).

Symmetry	Raman spectra			SERS
	Meilunas et al. (1991)	Lynch et al. (1995)	Luo and Yan (2005)	Luo and Yan (2005)
$A_g(1)$	496	496	497	491
$A_g(2)$	1470	1467	1467	1462



Zheng-Zhe Lin and Xi Chen, *Physics Letters A*, **377** (2013) 797-800.
H. Nejat Pishkenari and P. Ghaf Ghanbari, *Current Applied Physics*, **17** (2017) 72-77.
J. Du and P. Zeng. *European Journal of Mechanics A/Solids*, **28** (2009) 948–954.

Interatomic-potential-free Data-Driven molecular dynamics

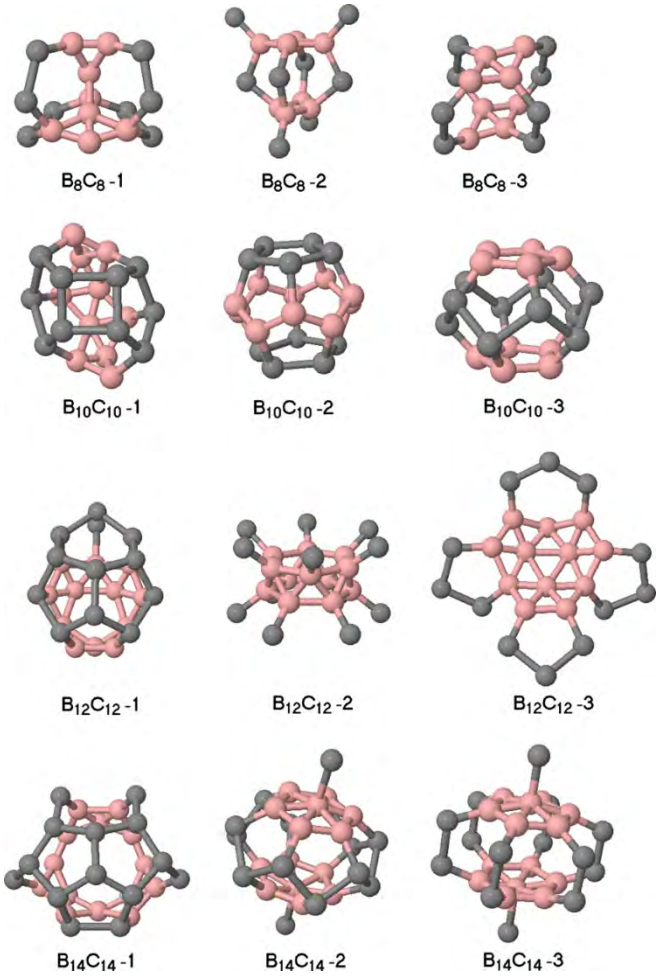
- Stillinger-Weber potential:

$$V_i = \sum_{j \in N_i} V_2(r_{ij}) + \sum_{\substack{j,k \in N_i \\ k>j}} V_3(r_{ij}, r_{ik}, \theta_{ijk}).$$

- Parameters for B and C from Dugan & Erkoc (2011).

Table 2
SW PEF parameters for carbon structures [31] (energies are in eV, distances are in Å).

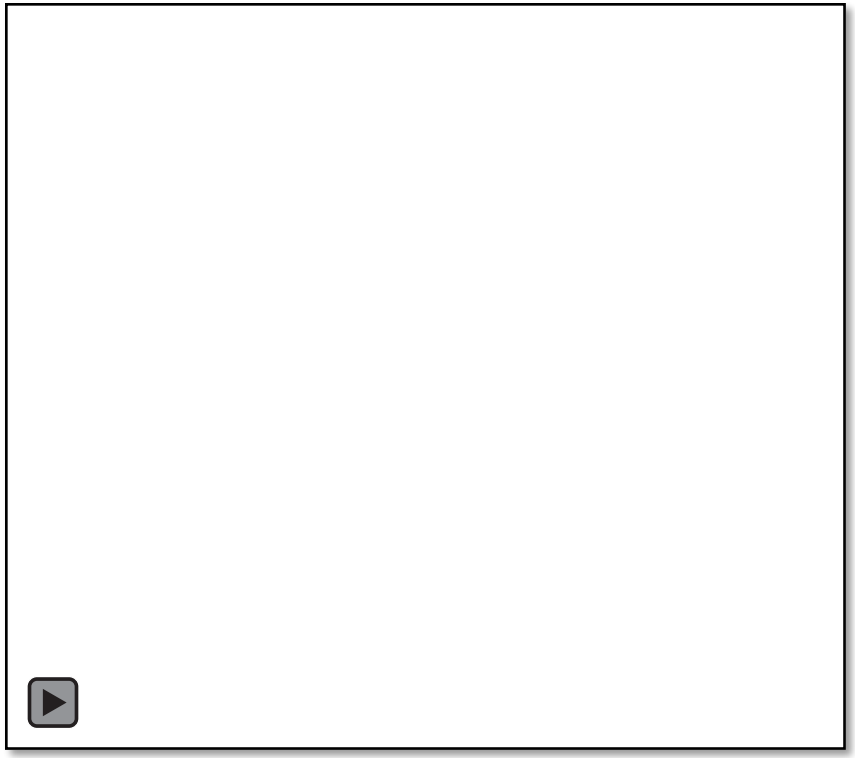
$A = 5.3790$
$B = 0.5082$
$b = 1.8945$
$\lambda = 18.7079$
$\gamma = 1.2$
$\kappa = 0.5$
$\sigma = 1.41800$



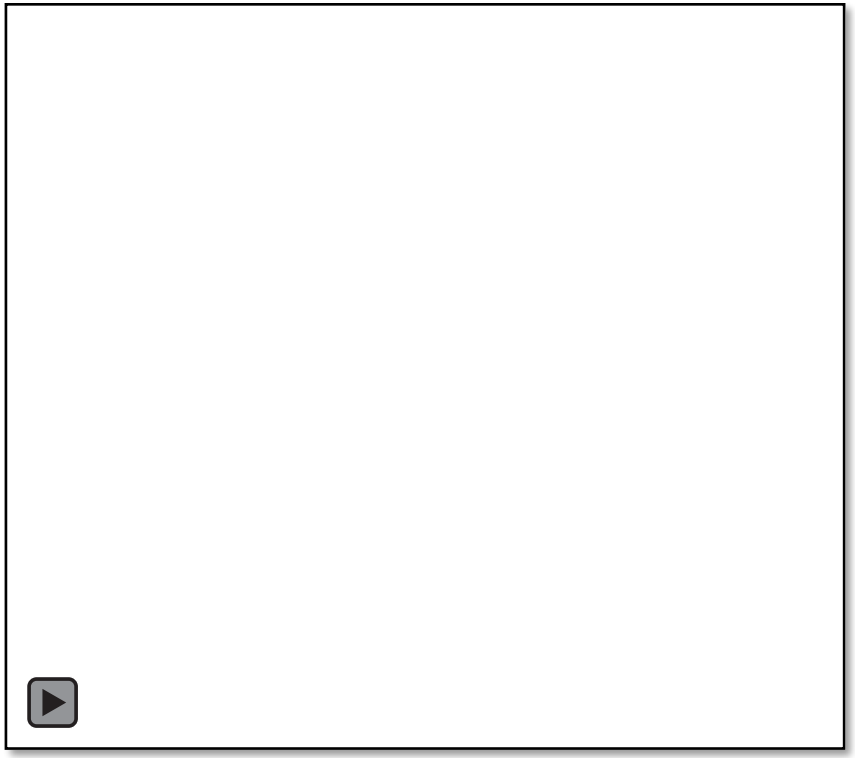
N. Dugan and S. Erkoç, *Computational Materials Science*, **50** (2011) 2950–2954.

Interatomic-potential-free Data-Driven molecular dynamics

- Ultrafast dynamics and fragmentation of C60 fullerene in intense laser pulses.



Converged Stillinger-Weber solution
at low amplitude (breathing mode)

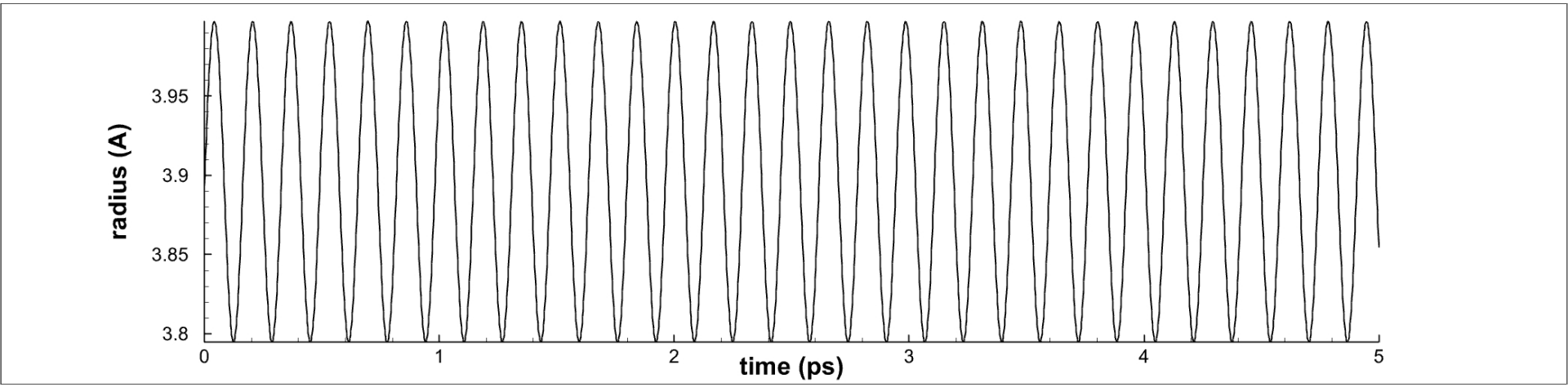


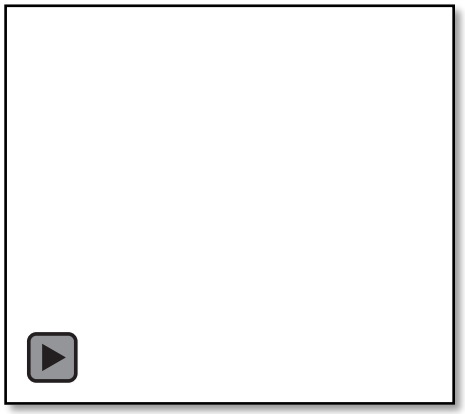
Converged Stillinger-Weber solution
at high amplitude (fragmetation)

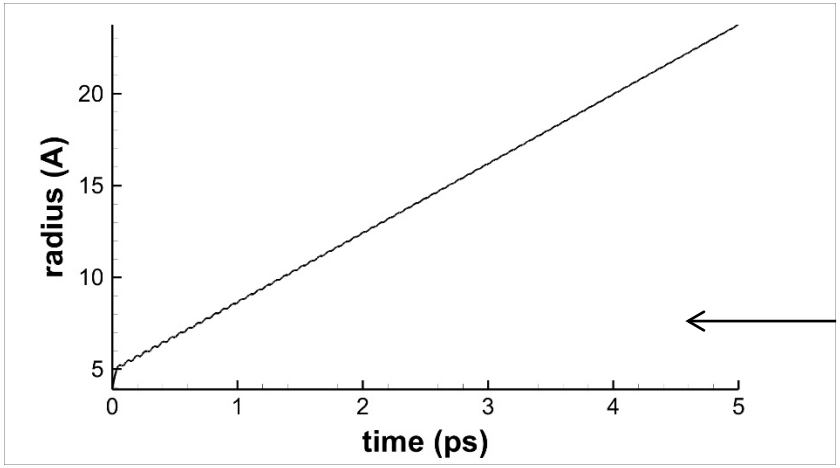
Bulin, J., Hamaeckers, J., Ariza, P. and Ortiz, M., arXiv:2208.04937

Interatomic-potential-free Data-Driven molecular dynamics

- Ultrafast dynamics and fragmentation of C60 fullerene in intense laser pulses.







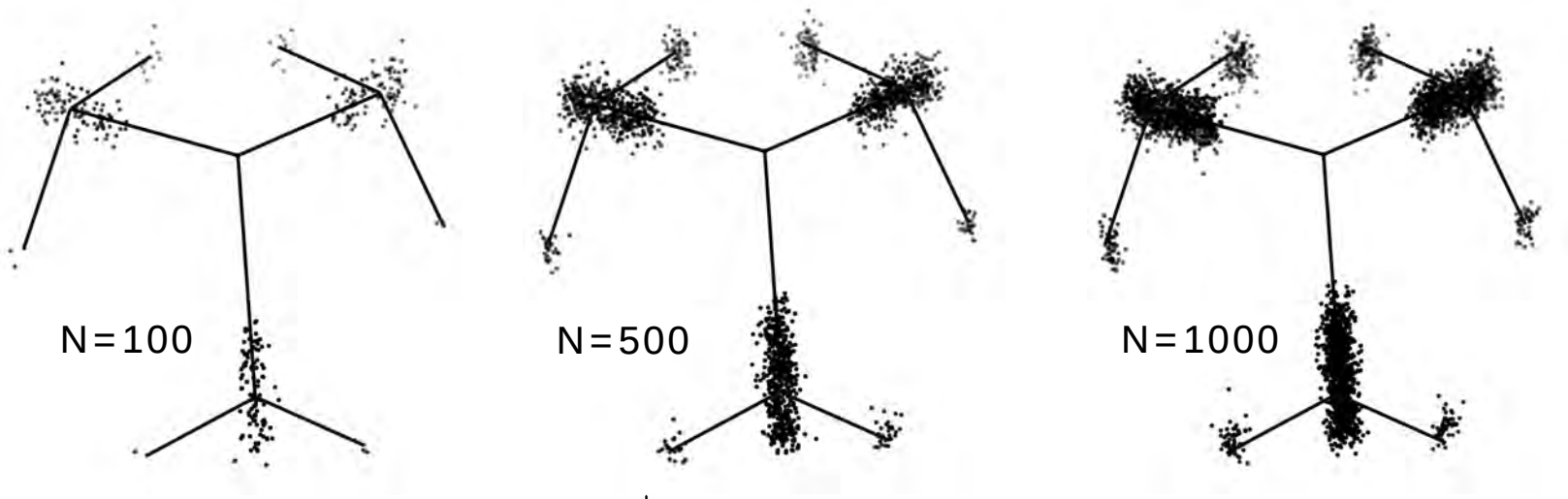
Converged Stillinger-Weber solution at low amplitude (breathing mode)

Converged Stillinger-Weber solution at high amplitude (fragmentation)

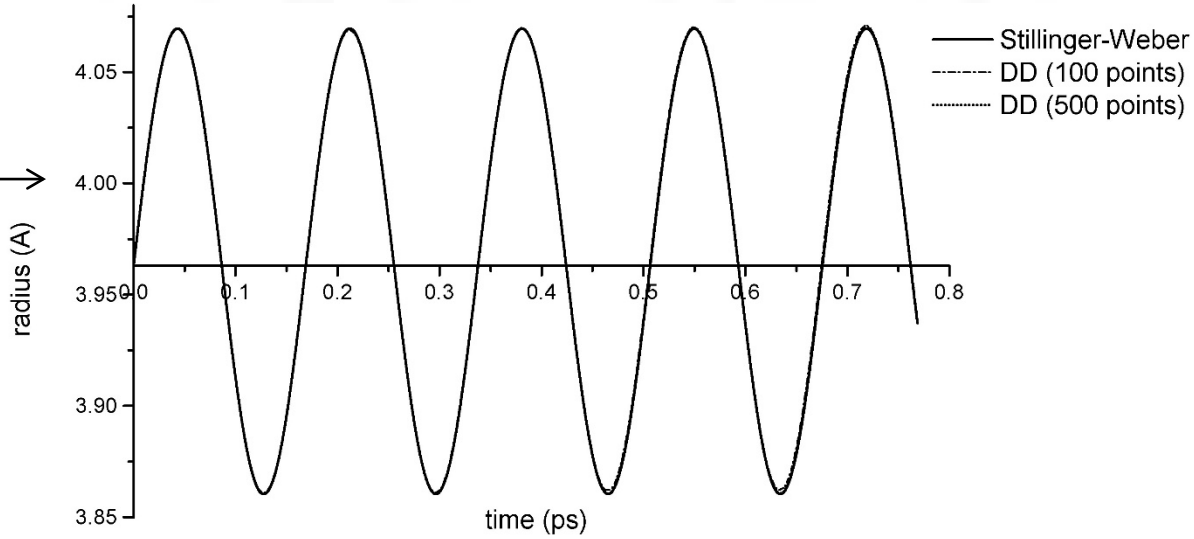
Bulin, J., Hamaeckers, J., Ariza, P. and Ortiz, M., arXiv:2208.04937

Interatomic-potential-free Data-Driven molecular dynamics

- Data sets sampled from Stillinger-Weber potential for use in Data-Driven Verlet calculations of ultrafast C60 fullerene at low amplitude.



Data-Driven Verlet solutions at low amplitude (breathing) demonstrating ***convergence for small-sized data sets!***
NB: ***No empirical potential*** is used at any point of the Data-Driven calculations!



Bulin, J., Hamaeckers, J., Ariza, P. and Ortiz, M., arXiv:2208.04937

Interatomic-potential-free Data-Driven molecular dynamics

- Generating good force-field data *a priori* may be challenging.
- Active learning: Exploit the variational structure of the Data-Driven solver to determine when new force-field data need to be acquired *ab initio*.
- Query strategy: Select for evaluation new computed local configurations that wander off from current data set by more than a given tolerance ε.

Algorithm Explicit Data-Driven dynamics with active learning

Require: Time step τ; arrays r_{k-1}, r_k, σ_k and f_k^{ext}; local force-field data sets D_i, sampling tolerance ε. Then:

i) Compute r_{k+1} from: $\displaystyle M\frac{r_{k+1}-2r_k+r_{k-1}}{\tau^2}+\sum_{i=1}^{n}B_i^T\sigma_{i,k}=f_k^{\text{ext}}$.

ii) Update strains: Set $\epsilon_{i,k+1}=B_i r_{k+1}$.

iii) Find $(\alpha_{i,k+1},\beta_{i,k+1})$ in D_i such that $\alpha_{i,k+1}$ is closest to $\epsilon_{i,k+1}$.

if $\text{dist}(\alpha_{i,k+1},\epsilon_{i,k+1})<\varepsilon$ **then**

iv.a) Update stresses: Set $\sigma_{i,k+1}=\beta_{i,k+1}$.

else

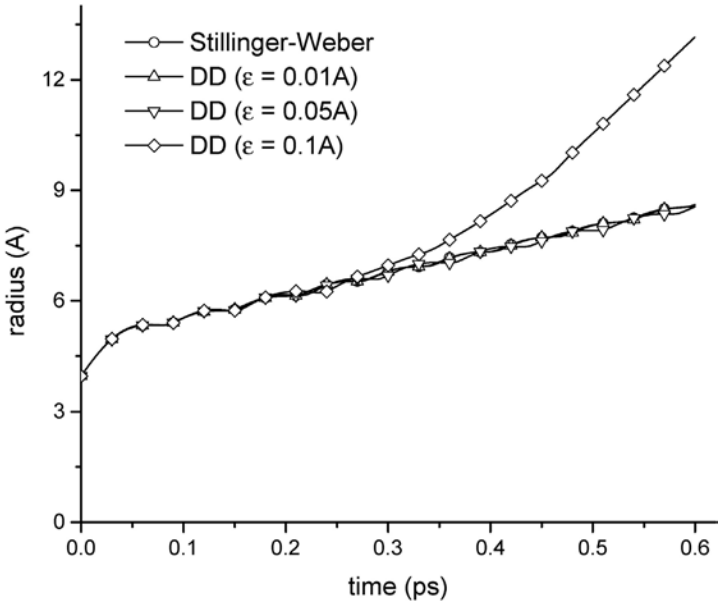
iv.b) Update data set: Compute $\sigma_{i,k+1}=\hat{\sigma}_i(\epsilon_{i,k+1})$, add $(\epsilon_{i,k+1},\sigma_{i,k+1})$ to D_i.

end if

v) Return r_k, r_{k+1}, σ_{k+1} and f_{k+1}^{ext}.

Interatomic-potential-free Data-Driven molecular dynamics

- Data-Driven Verlet calculations of ultrafast C60 fullerene at high amplitude (fragmentation) with adaptive learning.



- Number of force-evaluations for different values of the distance tolerance ε:

Stillinger-Weber	DD ($\varepsilon = 0.1$Å)	DD ($\varepsilon = 0.05$Å)	DD ($\varepsilon = 0.01$Å)
6000	269	370	1460

- The Data-Driven Verlet solutions converge robustly as ε is decreased.
- Convergence is achieved for modest data set sizes, without recourse to modeling!

to be continued...