Exactly Bit-Reversible Computational Methods for Memory-Efficient Adjoint Sensitivity Analysis of Dissipative Dynamic Systems

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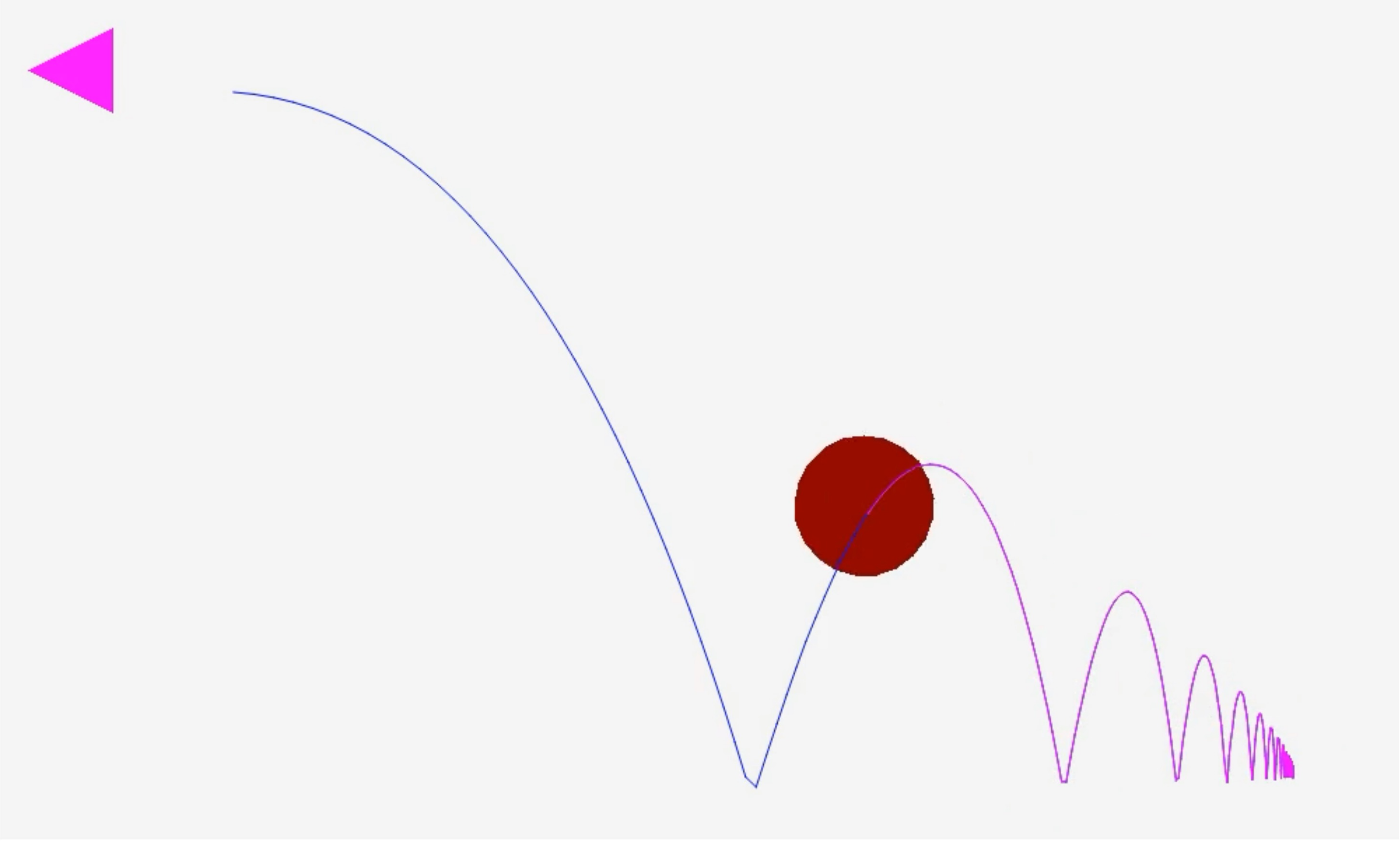
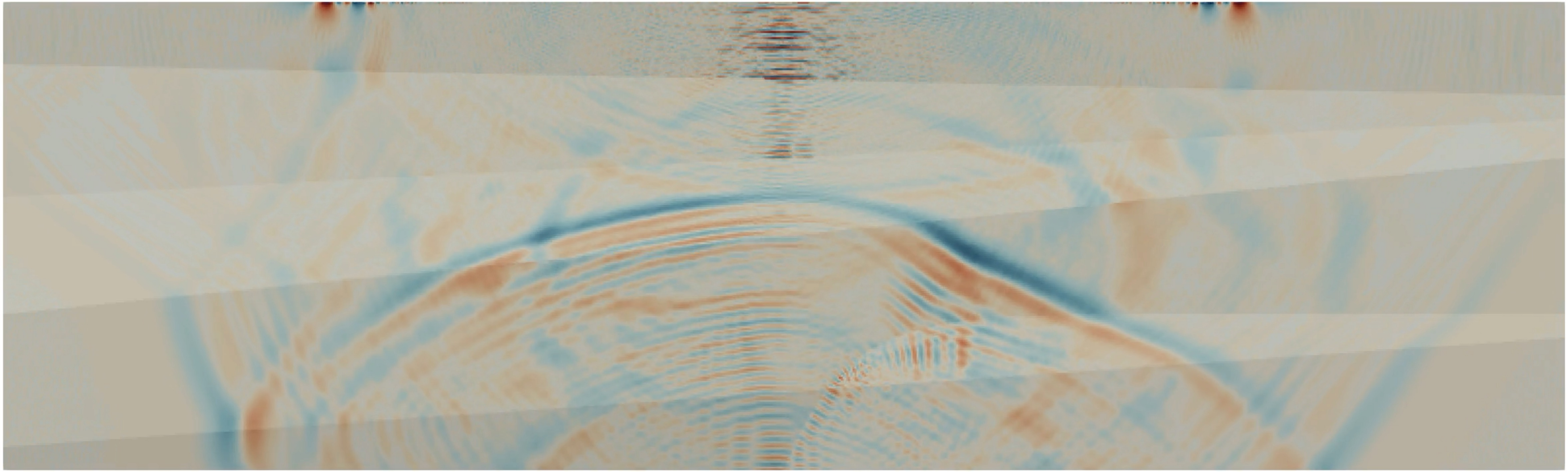
Computational Methods for Inverse Problems and Optimal Experimental Design



The adjoint state method provides an accurate and efficient means of computing sensitivities for dynamic optimization and inverse problems

Forward problem

t



$-t$

Adjoint problem

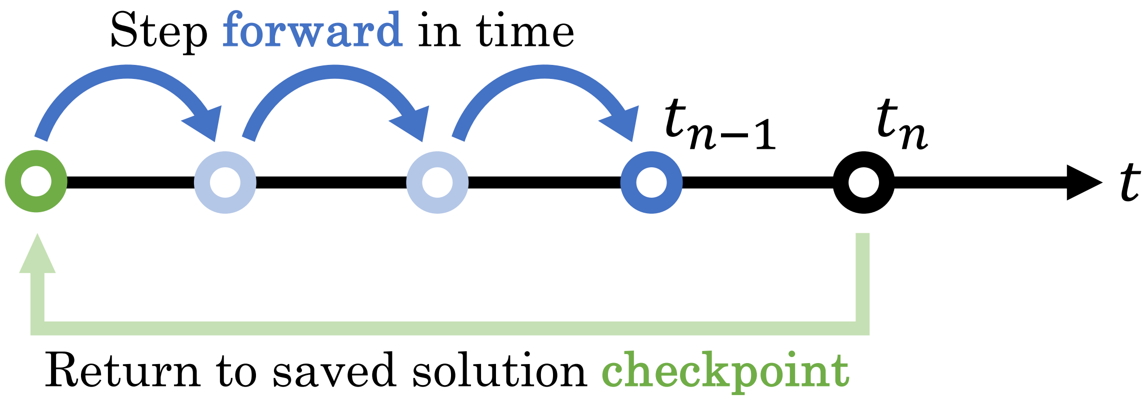
Common implementations of the discrete adjoint method use checkpointing to rematerialize forward solution states necessary for backpropagation

Solution of the adjoint problem must:

- *Store the forward solution* at all prior time states (more memory), or …
- *Rematerialize forward solution* from "checkpoints" (more computations)

Forward update:

$$\boldsymbol{u}_n = \boldsymbol{f}(\boldsymbol{u}_{n-1})$$



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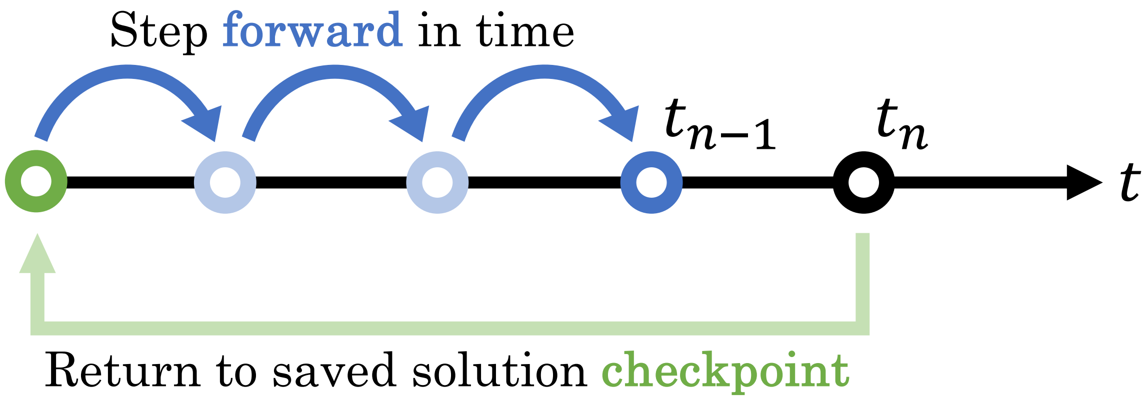


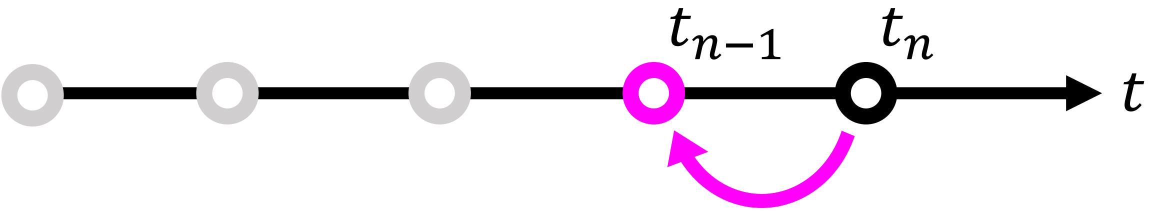
What if we could go *backwards* in time?

Hypothetical solution:

- *Reverse the computations*,
  and recover forward solution at each preceding step
- Requires *minimal memory and recomputation*

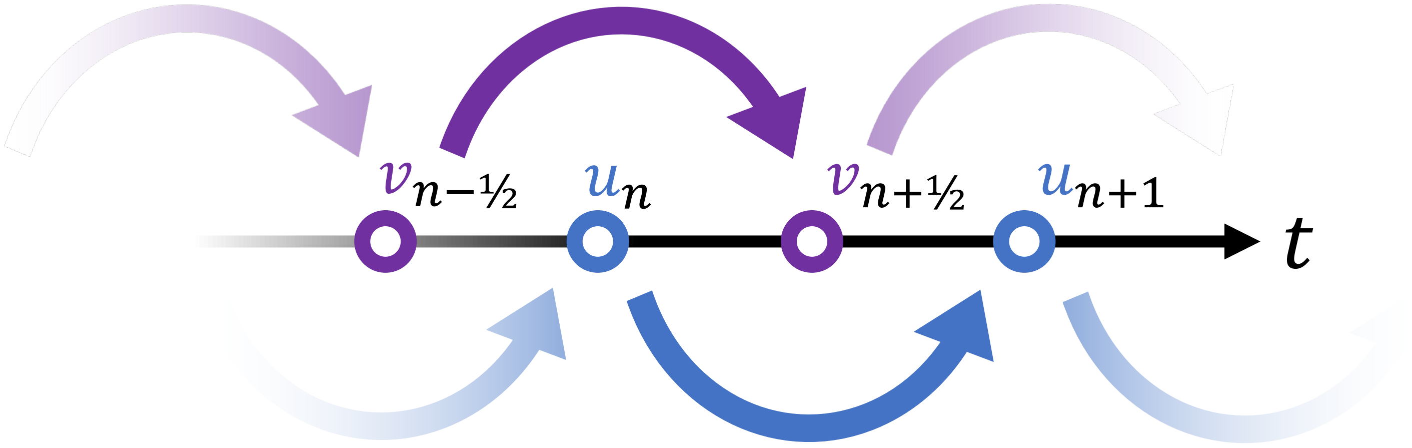
Backward update:

$$\boldsymbol{u}_{n-1} = \boldsymbol{f}^{-1}(\boldsymbol{u}_n)$$



Reverse computations to
step **backwards** in time

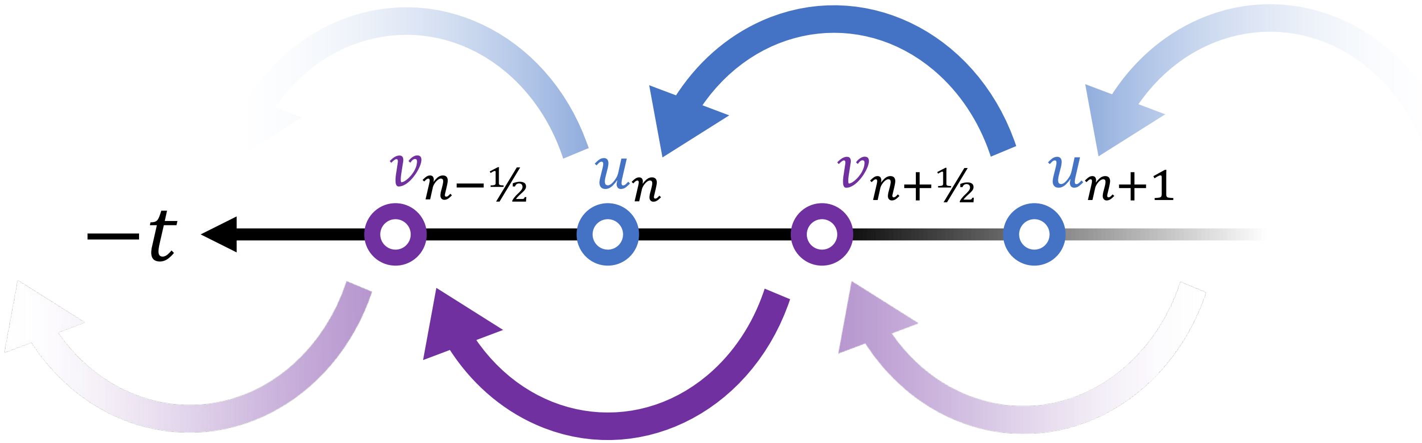
The leapfrog time-integrator is trivially reversible for Hamiltonian systems



Forward update:

$$v_{n+½} \leftarrow v_{n-½} + a(u_n)\Delta t$$

$$u_{n+1} \leftarrow u_n + v_{n+½}\Delta t$$



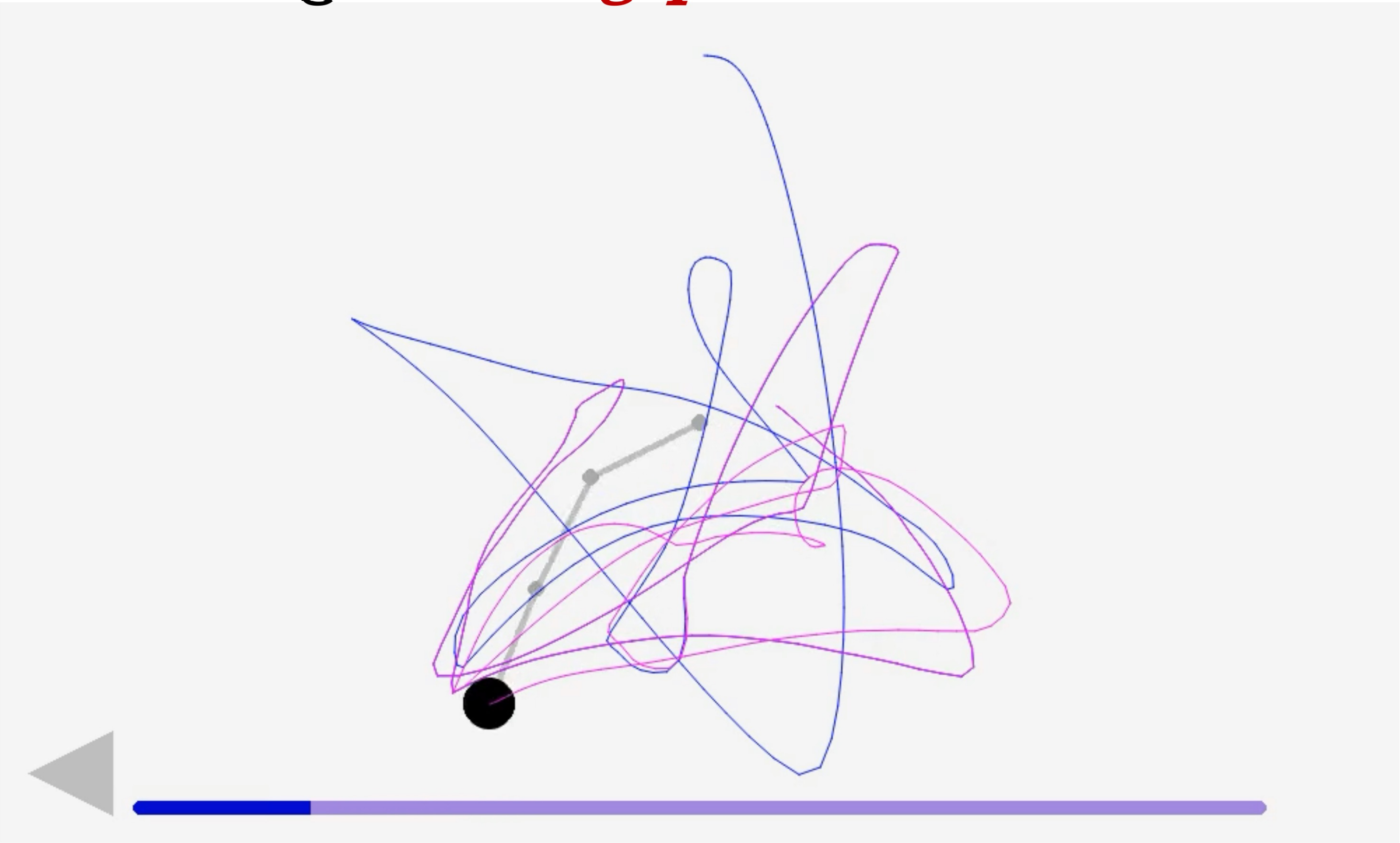
Backward update:

$$u_n \leftarrow u_{n+1} - v_{n+½}\Delta t$$

$$v_{n-½} \leftarrow v_{n+½} - a(u_n)\Delta t$$

Naïve time-reversal leads to inexact rematerialization due to round-off errors from *floating-point arithmetic*

Using *floating-point arithmetic*:



Forward update:

$$v_{n+1/2} \leftarrow v_{n-1/2} + a(u_n)\Delta t$$

$$u_{n+1} \leftarrow u_n + v_{n+1/2}\Delta t$$

Backward update:

$$u_n \leftarrow u_{n+1} - v_{n+1/2}\Delta t$$

$$v_{n-1/2} \leftarrow v_{n+1/2} - a(u_n)\Delta t$$

Represent displacement and velocity degrees of freedom as fixed-width (32- or 64-bit) integers with implied (but differing) problem-dependent radices

mantissa radix exponent

Fixed $x \in \mathbb{R}$ $\quad$ $x = m \times \underbrace{R^e}_{\textit{fixed}}$ $\quad$ **Integer** $m \in \mathbb{Z}$

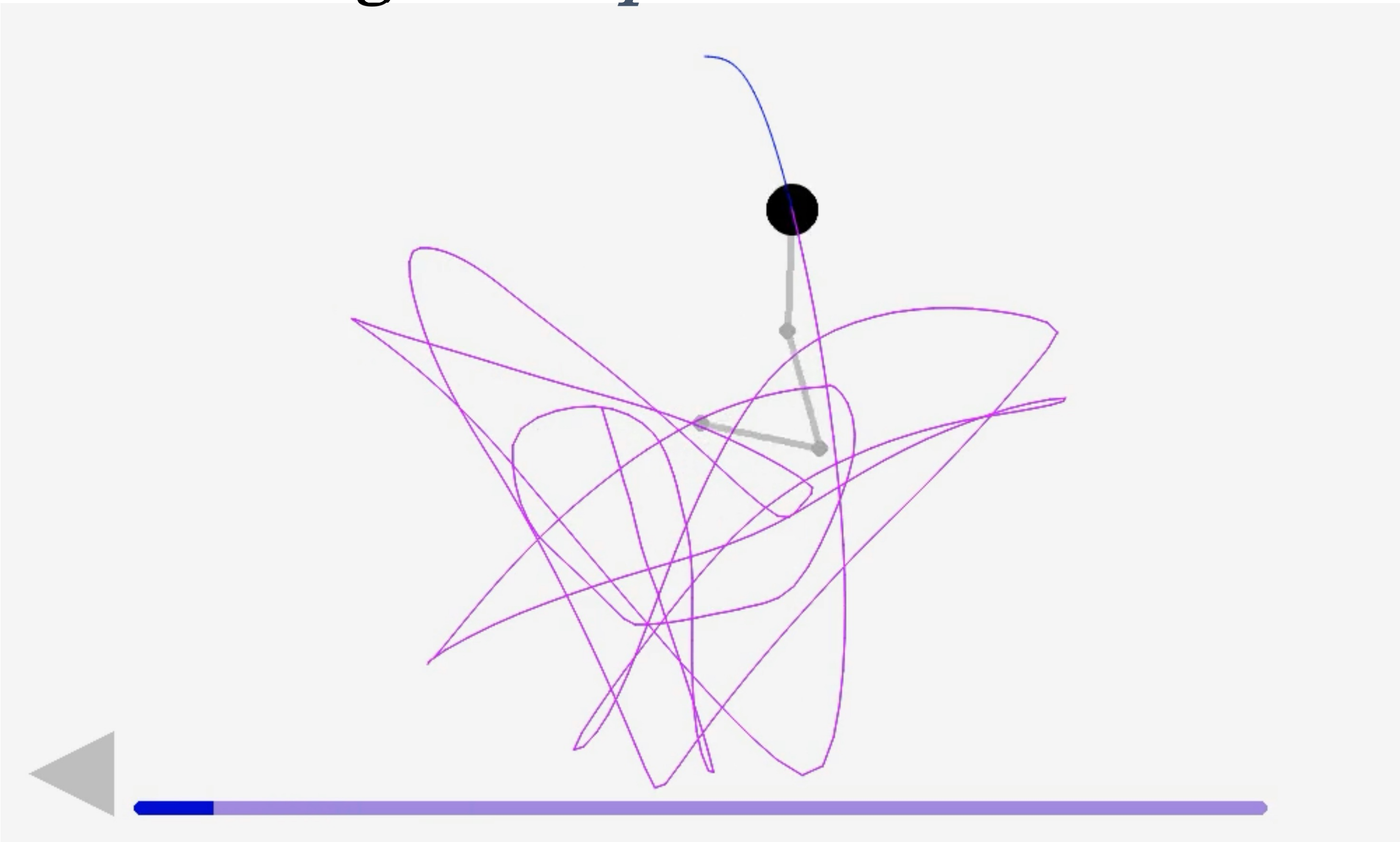
e.g. $\quad 7.560239 = 7560239 \times 10^{-6}$

$x \in [-2147.483648, +2147.483647]$ (32-bit int)

$x \in [-9.223 \ldots \times 10^{12}, +9.223 \ldots \times 10^{12}]$ (64-bit int)

Round-off errors from addition/subtraction can be eliminated using *fixed-point arithmetic*, resulting in exactly "bit-reversible" time-integration

Using *fixed-point arithmetic*:

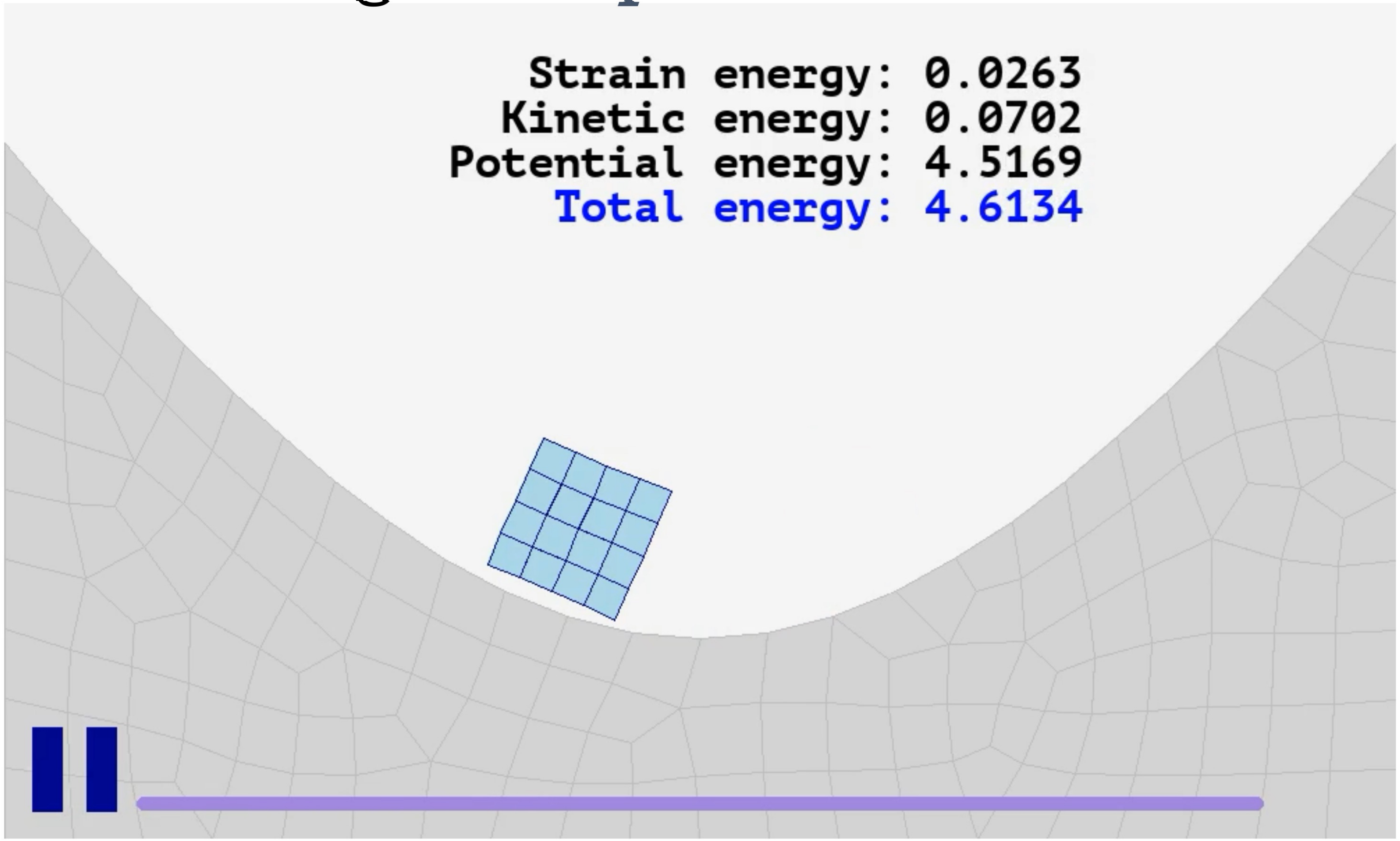


Idea previously applied to:

- **Molecular dynamics** (Levesque and Verlet, 1993)
- **Continuum mechanics** (Kum and Hoover, 1994)
- **N-body simulations** (Rein and Tamayo, 2017)
- **Chaotic dynamic systems** (Jos Stam, 2022) josstam.com/reversible

For *dissipative* dynamic systems (with damping), fixed precision arithmetic alone is insufficient to ensure exact bit-reversibility

Using *fixed-point arithmetic*:



$$\boldsymbol{M}\ddot{u} + \boldsymbol{C}\dot{u} + \boldsymbol{K}u = \boldsymbol{F}$$

damping

$$v_n \leftarrow v_{n-½} + a(u_n)\Delta t/2$$

$$v_n \leftarrow v_n \times \frac{M - C\Delta t/2}{M + C\Delta t/2}$$

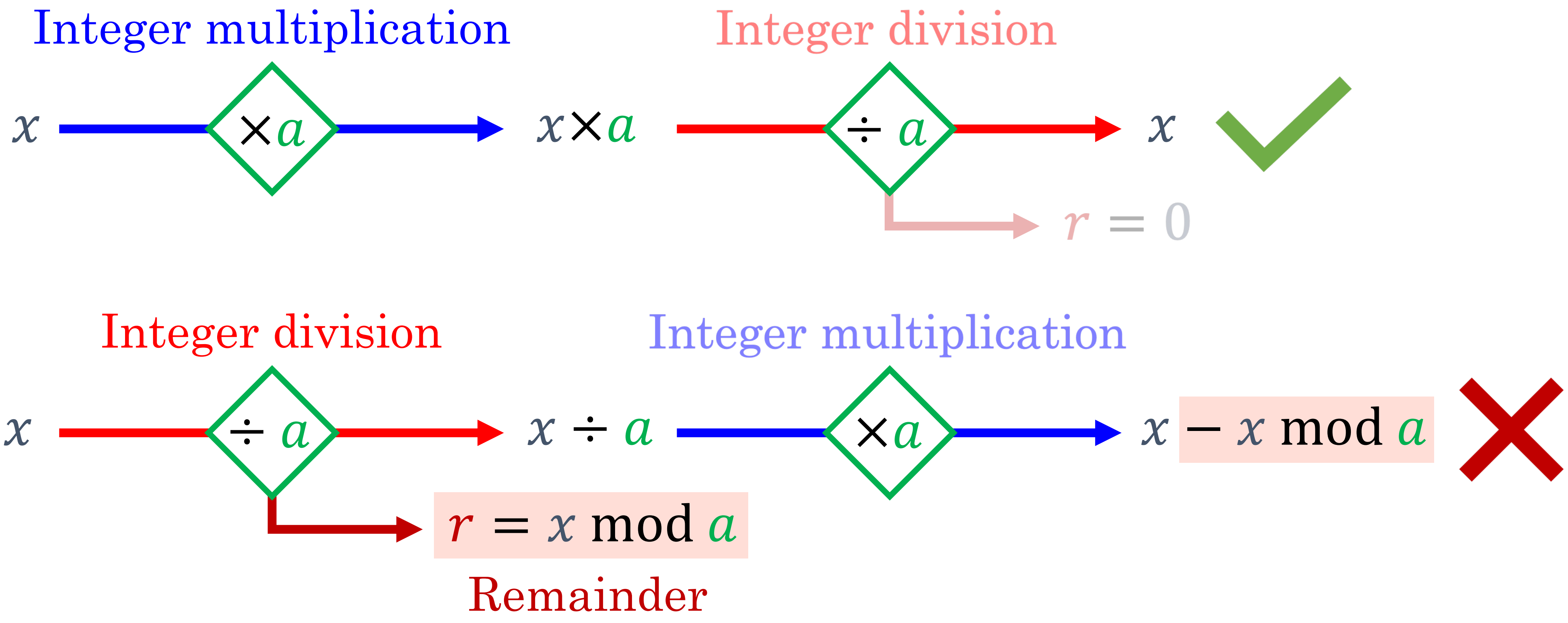
$$v_{n+½} \leftarrow v_n + a(u_n)\Delta t/2$$

$$u_{n+1} \leftarrow u_n + v_{n+½}\Delta t$$

Addition/subtraction: *reversible*

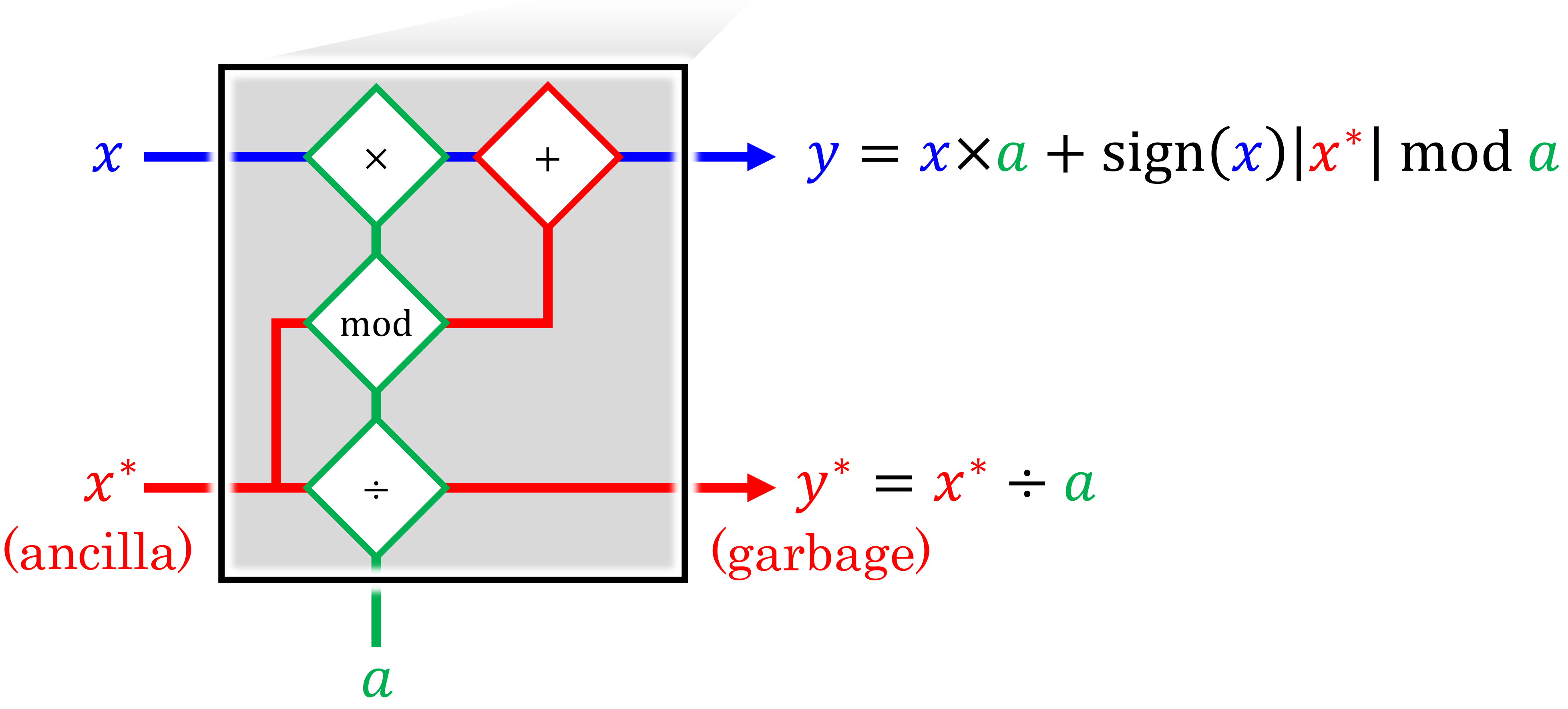
Multiplication/division: *not reversible*

Euclidean division of integers results in permanent loss (“dissipation”) of information in the form of the *remainder* after division



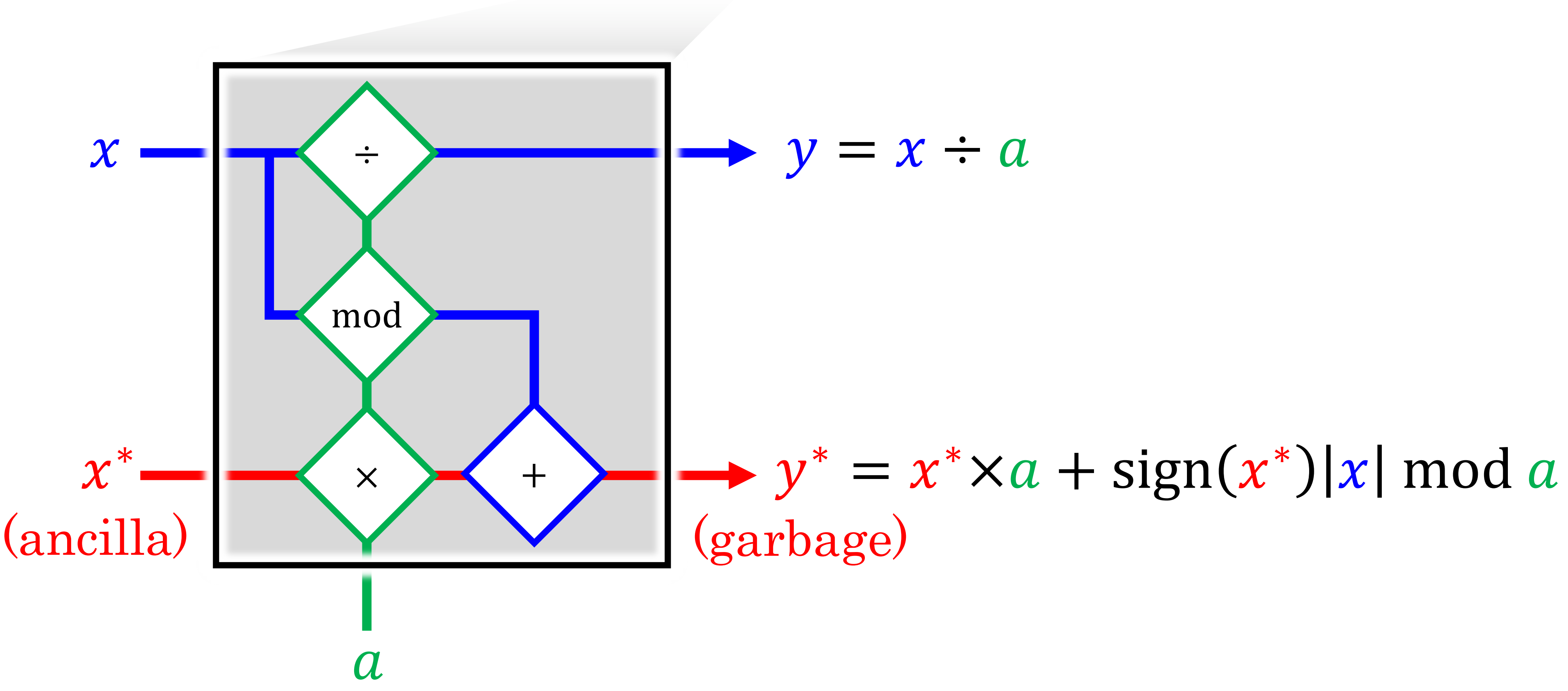
Use the round-off bit buffering approach proposed by Maclaurin et al. (2015) to define a *paired integer multiplication/division operation*

$$(x, x^*)[\times, \div]a = (y, y^*)$$



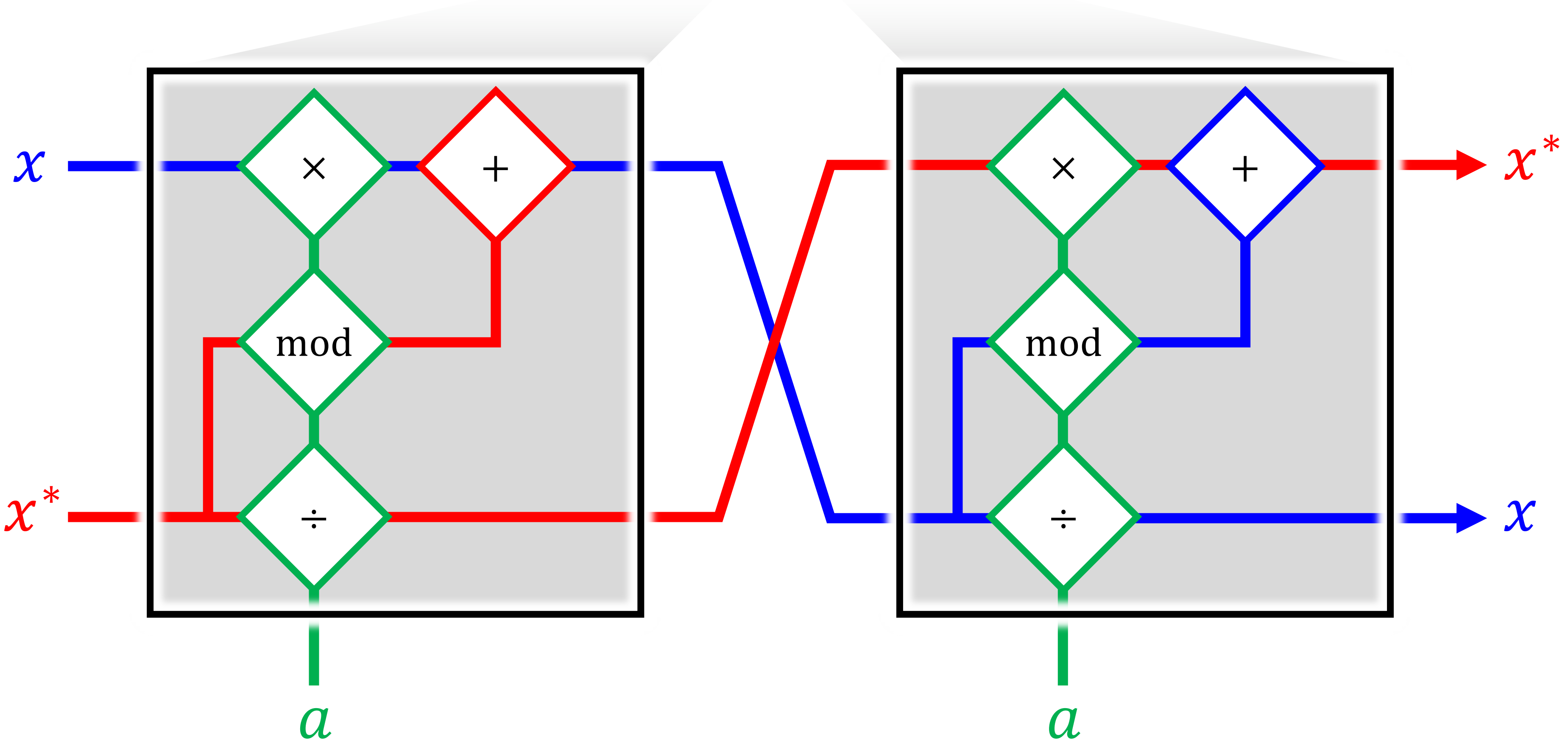
The inverse paired division/multiplication operation is obtained by simply permuting the inputs

$$(x, x^*)[\div,\times]a = (y, y^*)$$



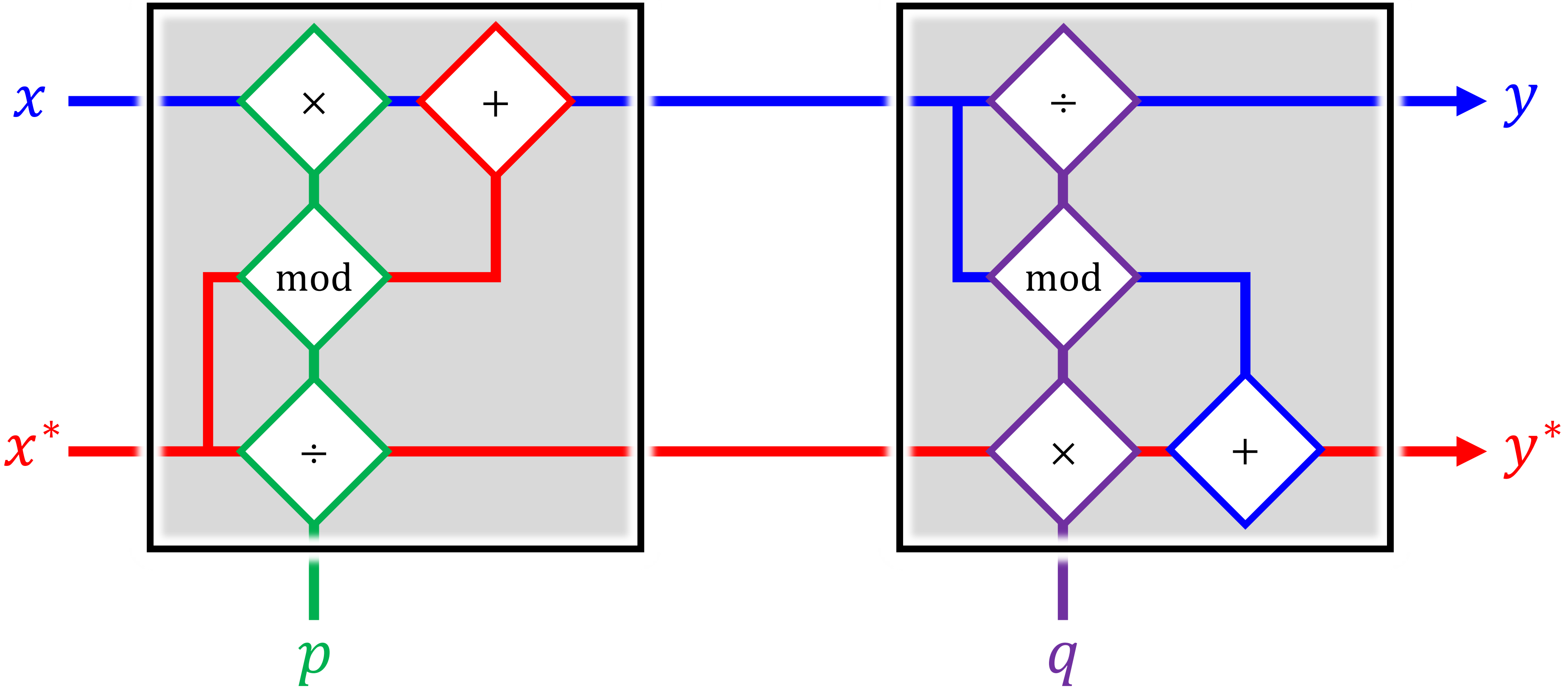
The paired integer multiplication/division operation and its permuted inverse are *exactly bit-reversible*

$$\big((x, x^*)[\times,\div]a\big)[\div,\times]a = (x, x^*)$$



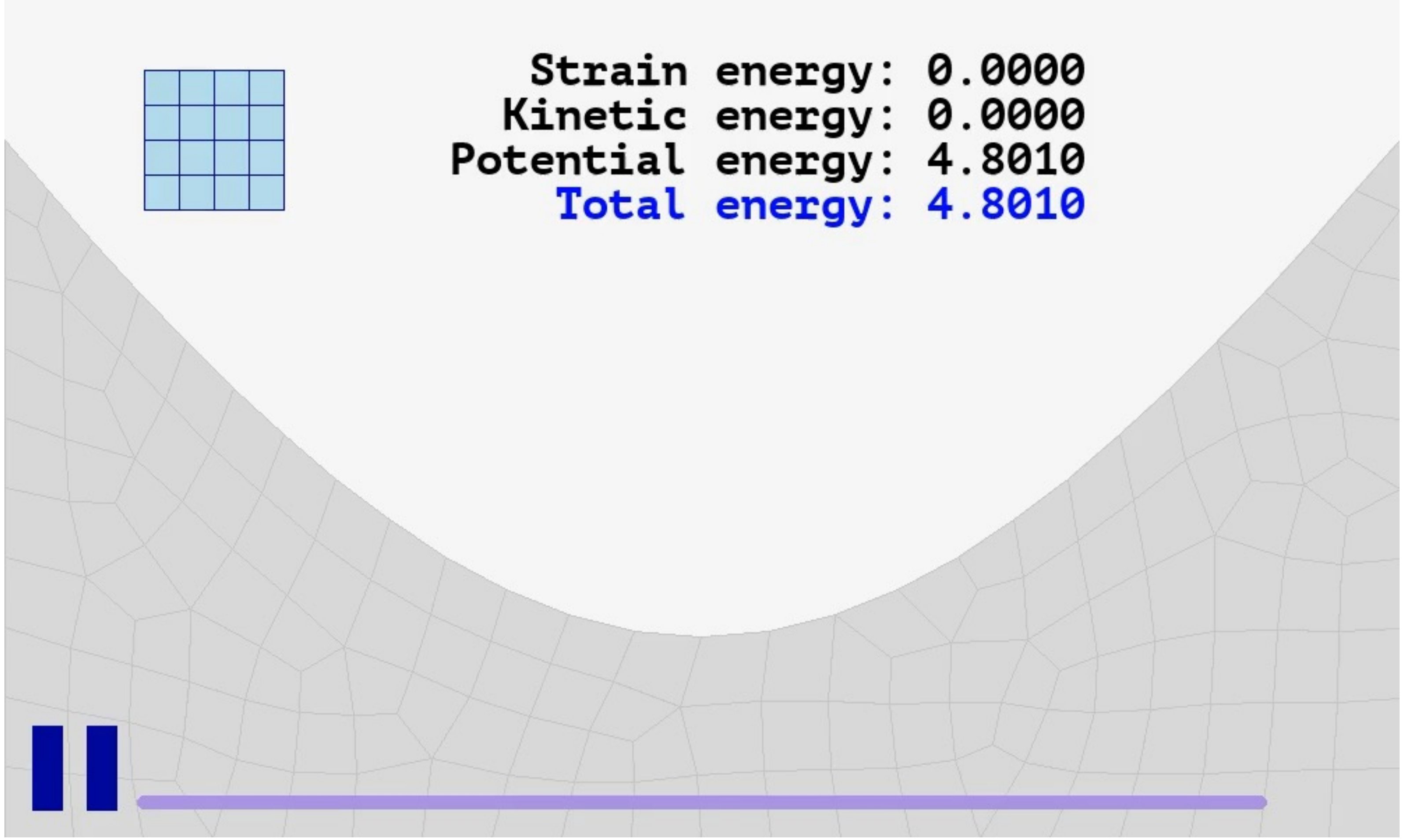
Bit-reversible fixed-point multiplication is carried out by approximating the multiplicand as a *rational number*

$$(x, x^*)[\times,\div]\frac{p}{q} = ((x, x^*)[\times,\div]p)[\div,\times]q = (y, y^*)$$



Using *paired integer multiplication/division* ensures bit-reversibility for dissipative dynamic systems

Using *paired integer multiplication/division*:



$$M\ddot{u} + C\dot{u} + Ku = F$$

mass-proportional damping:

$$C = \alpha M$$

$$v_n \leftarrow v_{n-½} + a(u_n)\Delta t/2$$

$$(v_n, v_{n+1}^*) \leftarrow (v_n, v_n^*)[\times,\div]\frac{1-\alpha\Delta t/2}{1+\alpha\Delta t/2}$$

$$v_{n+½} \leftarrow v_n + a(u_n)\Delta t/2$$

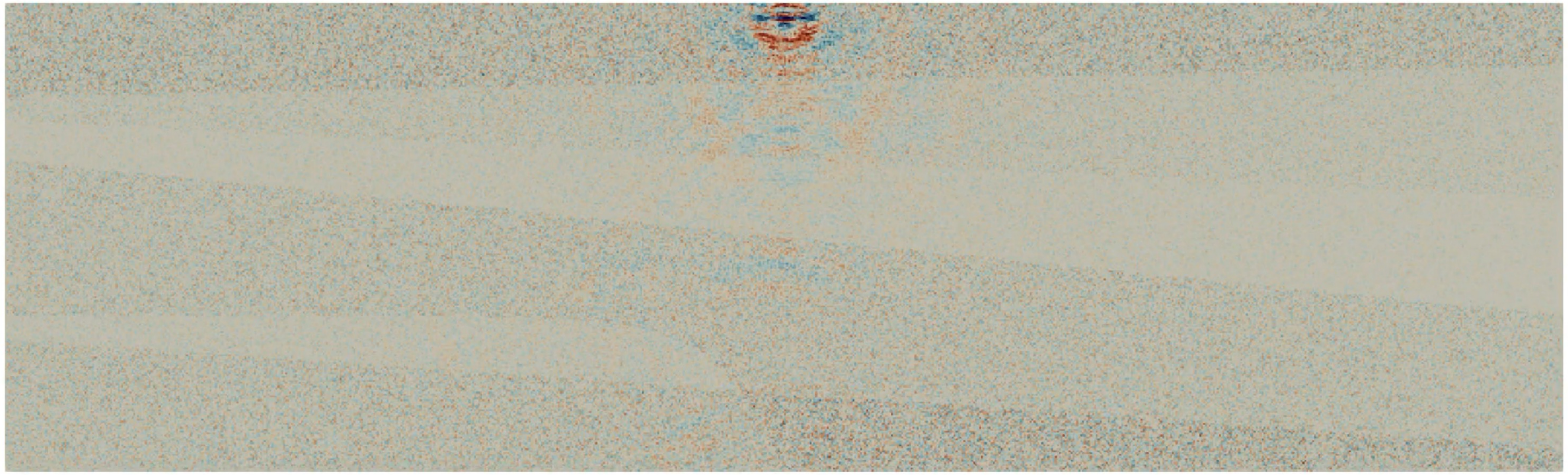
$$u_{n+1} \leftarrow u_n + v_{n+½}\Delta t$$

Ancilla velocity state variables: v_n^*

Addition/subtraction: *reversible*

Paired multiplication/division: *reversible*

Using *paired integer multiplication/division* ensures bit-reversibility for dissipative dynamic systems



Fixed-point arithmetic

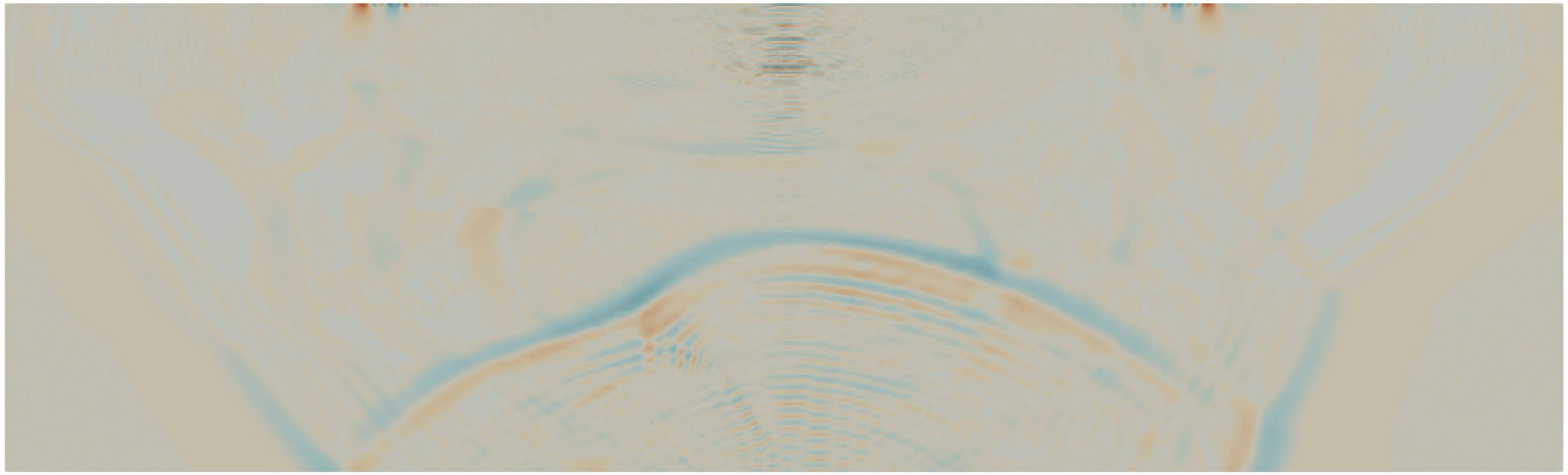
unpaired integer multiplication/division (*not* reversible)

Fixed-point arithmetic

paired integer multiplication/division (reversible)

386k degrees of freedom 1000 time steps

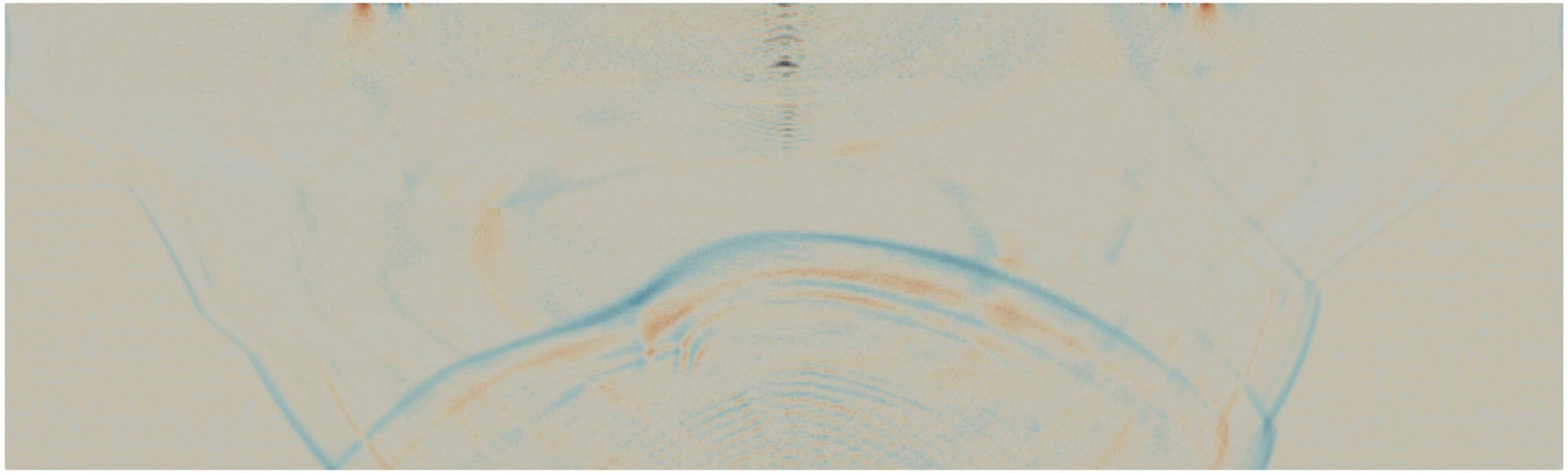
Forward solution accuracy, memory, and run-time performance using paired fixed-point arithmetic is comparable to that of floating-point arithmetic



Floating-point

1×{64-bit float (double)}

Run-time: 47.3 s



Fixed-point (reversible)

2×{32-bit int}

Run-time: 50.2 s

(6% slower)

386k degrees of freedom 1000 time steps

The concept of bit-reversible scalar multiplication/division can be generalized to achieve bit-reversible *matrix multiplication/inversion*

$$\boldsymbol{A} = \boldsymbol{LDU}$$

$$\boldsymbol{L} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ L_{21} & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ L_{N1} & L_{N2} & \cdots & 1 \end{bmatrix} \quad \boldsymbol{D} = \begin{bmatrix} D_{11} & 0 & \cdots & 0 \\ 0 & D_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & D_{NN} \end{bmatrix} \quad \boldsymbol{U} = \begin{bmatrix} 1 & U_{12} & \cdots & U_{1N} \\ 0 & 1 & \cdots & U_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix}$$

$$D_{ii} \approx \frac{b_i}{d_i} \in \mathbb{Q}$$

$\forall i = 1, \ldots, N$ $\qquad\qquad$ $\forall i = N, \ldots, 1$

$$\boxed{y_i = \hat{y}_i + \textstyle\sum_{j<i} L_{ij}\hat{y}_j} \Leftarrow \boxed{(\hat{y}_i, \hat{y}_i^*) = (\hat{x}_i, \hat{x}_i^*)[\times, \div]\frac{b_i}{d_i}} \Leftarrow \boxed{\hat{x}_i = x_i + \textstyle\sum_{j>i} U_{ij} x_j}$$

$$\underbrace{\boldsymbol{y} = \boldsymbol{L}\hat{\boldsymbol{y}} \qquad \hat{\boldsymbol{y}} = \boldsymbol{D}\hat{\boldsymbol{x}} \qquad \hat{\boldsymbol{y}}^* = \hat{\boldsymbol{x}}^*\boldsymbol{D}^{-1} \qquad \hat{\boldsymbol{x}} = \boldsymbol{U}\boldsymbol{x}}_{\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}}$$

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$\forall i = 1, \ldots, N$ $\qquad$ $\forall i = N, \ldots, 1$

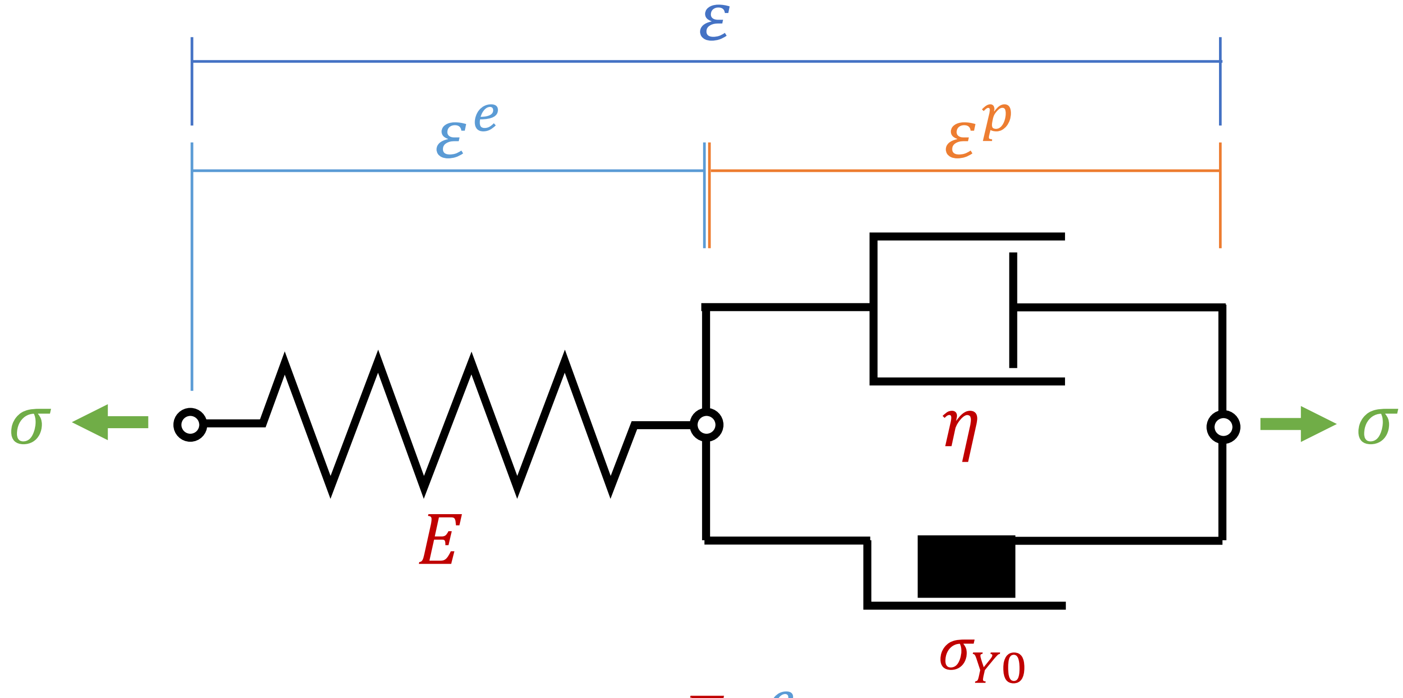
$$\boxed{\hat{y}_i = y_i - \sum_{j<i} L_{ij}\hat{y}_j} \Rightarrow \boxed{(\hat{x}_i, \hat{x}_i^*) = (\hat{y}_i, \hat{y}_i^*)[\div,\times]\frac{b_i}{d_i}} \Rightarrow \boxed{x_i = \hat{x}_i - \sum_{j>i} U_{ij}x_j}$$

$$\hat{\boldsymbol{y}} = \boldsymbol{L}^{-1}\boldsymbol{y} \qquad \hat{\boldsymbol{x}} = \boldsymbol{D}^{-1}\hat{\boldsymbol{y}} \qquad \hat{\boldsymbol{x}}^* = \hat{\boldsymbol{y}}^*\boldsymbol{D} \qquad \boldsymbol{x} = \boldsymbol{U}^{-1}\hat{\boldsymbol{x}}$$

$$\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{y}$$

The proposed set of bit-reversible operations can be used to implement reversible time-integrators for common visco-elastic/plastic constitutive models

Bingham-Maxwell Model:



$$\sigma = E\varepsilon^e$$

$$|\sigma - \eta\dot{\varepsilon}^p| \leq \sigma_{Y0}$$

$$\lambda = e^{-E\Delta t/\eta}$$

$$\varepsilon_0^p = \varepsilon - \mathrm{sign}(\varepsilon - \varepsilon^p)\sigma_{Y0}/E$$

Forward:

If $|E(\varepsilon - \varepsilon^p)| > \sigma_{Y0}$

$$(\varepsilon^p, \varepsilon^{p*}) \leftarrow (\varepsilon^p, \varepsilon^{p*})[\times, \div]\lambda$$

$$\varepsilon^p \leftarrow \varepsilon^p + \varepsilon_0^p(1 - \lambda)$$

Backward:

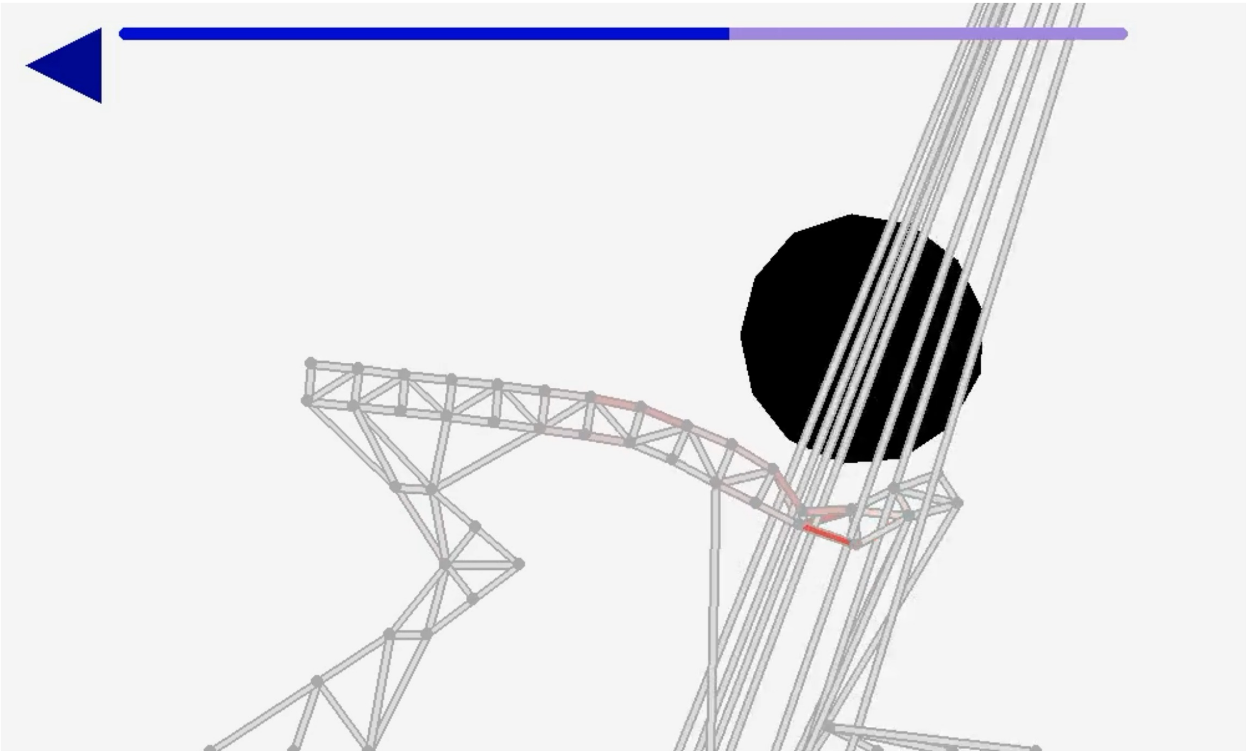
If $|E(\varepsilon - \varepsilon^p)| > \sigma_{Y0}$

$$\varepsilon^p \leftarrow \varepsilon^p - \varepsilon_0^p(1 - \lambda)$$

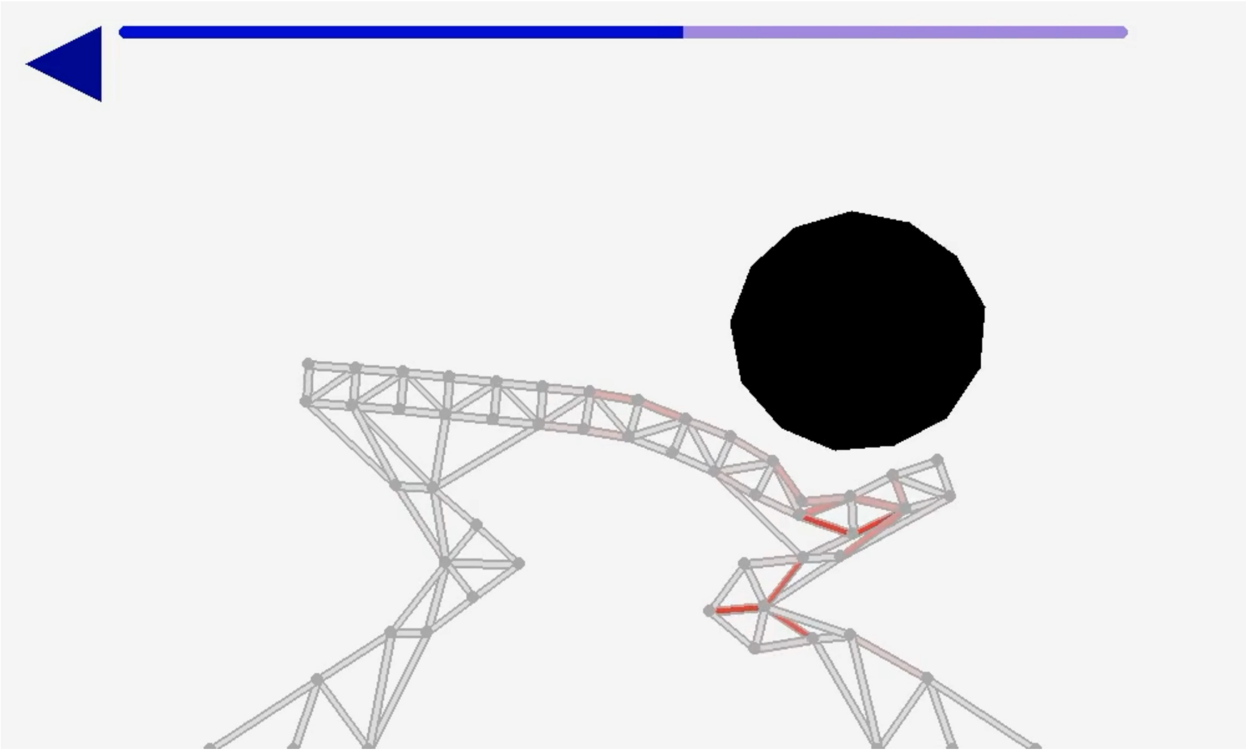
$$(\varepsilon^p, \varepsilon^{p*}) \leftarrow (\varepsilon^p, \varepsilon^{p*})[\div, \times]\lambda$$

Demonstration: implementation of a reversible uniaxial visco-plasticity model with a maximum plastic strain-based failure criterion

Floating-point (*not* reversible)



Fixed-point (reversible)



Ongoing and future work

- Limitations:
    - **Overflow**!
    - Not all models are amenable to a reversible implementation
    - Must ensure *consistent* execution during forward/backward passes
- Alternative bit-roundoff data compression methods
- Inelastic material behavior
    - Continuum damage/plasticity/visco-elasticity, fracture, friction
- Compare performance on GPUs
    - Does the proposed approach help with minimizing device I/O and latency?
- Application to optimization/inverse problems
    - Optimal design of impact-resistant structures

Questions?