QLB: Collision-Aware Quasi-Newton Solver with Cholesky and L-BFGS for Nonlinear Time Integration—Supplemental Document

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1 INTEGRATORS

In this section, we describe the various integrators we use to test the performance of our approach. Let $\mathbf{x}$ and $\mathbf{v}$ be the nodal positions and velocities of the volumetric solid, and $\mathbf{M}$ be the constant mass matrix. Furthermore, let $\mathbf{f}(\mathbf{x}, \mathbf{v})$ be the force vector, and derivatives $\mathbf{D} = d\mathbf{f}/d\mathbf{v}$ and $\mathbf{K} = d\mathbf{f}/d\mathbf{x}$ be the damping and stiffness matrices, respectively. Thus, the goal of each integrator is to compute the nodal positions $\mathbf{x}^{(k+1)}$ given $\mathbf{x}^{(k)}$. After computing $\mathbf{x}^{(k+1)}$, we compute the nodal velocities $\mathbf{v}^{(k+1)}$ using the discretization scheme of the particular integrator.

1.1 BDF1

With BDF1 (1st-order Backward Differentiation Formula) [Hairer et al. 2006], we solve a nonlinear system to advance the state from step k to $k + 1$:

$$\mathbf{M}\mathbf{v}^{(k+1)} = \mathbf{M}\mathbf{v}^{(k)} + h\mathbf{f}^{(k+1)} \tag{1a}$$

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + h\mathbf{v}^{(k+1)}, \tag{1b}$$

where h is the time step. Solving Eq. 1b for $\mathbf{v}^{(k+1)}$ and plugging the result into Eq. 1a, we get the following equation:

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + h\left(\mathbf{v}^{(k)} + h\mathbf{M}^{-1}\mathbf{f}^{(k+1)}\right). \tag{2}$$

We then multiply by $\mathbf{M}$ to get the following equation:

$$\mathbf{M}\mathbf{x}^{(k+1)} = \mathbf{M}\mathbf{x}^{(k)} + \mathbf{M}h\mathbf{v}^{(k)} + h^2\mathbf{f}^{(k+1)}, \tag{3}$$

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for which we wish to find a root $\mathbf{x}^{(k+1)}$. We do so using Newton's Method. After some rearranging, the Newton search direction for the nonlinear system becomes $\Delta\mathbf{x}_i = -\mathbf{H}_i^{-1}\mathbf{g}_i$, with

$$\begin{aligned} \mathbf{g}_i &= \mathbf{M}\left(\mathbf{x}_i^{(k+1)} - \mathbf{x}^{(k)} - h\mathbf{v}^{(k)}\right) - h^2\mathbf{f}_i^{(k+1)} \\ \mathbf{H}_i &= \mathbf{M} - h\mathbf{D}_i^{(k+1)} - h^2\mathbf{K}_i^{(k+1)}, \end{aligned} \tag{4}$$

where i indicates the current iteration of the nonlinear solve.

1.2 Quasistatic

The quasistatic time stepper solves the nonlinear system

$$\mathbf{f}^{(k+1)} = 0 \tag{5}$$

at each time step, with time-varying boundary conditions or forces. The Newton search direction for the nonlinear system is $\Delta\mathbf{x}_i = -\mathbf{H}_i^{-1}\mathbf{g}_i$, with

$$\begin{aligned} \mathbf{g}_i &= -\mathbf{f}_i^{(k+1)} \\ \mathbf{H}_i &= -\mathbf{K}_i^{(k+1)}. \end{aligned} \tag{6}$$

1.3 BDF2

With BDF2 (2nd-order Backward Differentiation Formula) [Hairer et al. 2006], we solve a nonlinear system to compute the state at $k+1$ using the states at $k-1$ and k:

$$\mathbf{M}\mathbf{v}^{(k+1)} = \frac{4}{3}\mathbf{M}\mathbf{v}^{(k)} - \frac{1}{3}\mathbf{M}\mathbf{v}^{(k-1)} + \frac{2}{3}h\mathbf{f}^{(k+1)} \tag{7a}$$

$$\mathbf{x}^{(k+1)} = \frac{4}{3}\mathbf{x}^{(k)} - \frac{1}{3}\mathbf{x}^{(k-1)} + \frac{2}{3}h\mathbf{v}^{(k+1)}. \tag{7b}$$

Using a similar process to the one in §1.1, the Newton search direction for the nonlinear system becomes $\Delta\mathbf{x}_i = -\mathbf{H}_i^{-1}\mathbf{g}_i$, with

$$\begin{aligned} \mathbf{g}_i &= \mathbf{M}\left(\mathbf{x}_i^{(k+1)} - \frac{4}{3}\mathbf{x}^{(k)} + \frac{1}{3}\mathbf{x}^{(k-1)} - \frac{8}{9}h\mathbf{v}^{(k)} + \frac{2}{9}h\mathbf{v}^{(k-1)}\right) - \frac{4}{9}h^2\mathbf{f}_i^{(k+1)} \\ \mathbf{H}_i &= \mathbf{M} - \frac{2}{3}h\mathbf{D}_i^{(k+1)} - \frac{4}{9}h^2\mathbf{K}_i^{(k+1)}. \end{aligned} \tag{8}$$

On the very first time step, we cannot use BDF2 since it requires solutions at two previous time steps. Instead, we use SDIRK2, described below, to start BDF2 [Nishikawa 2019].

1.4 SDIRK2

With SDIRK2 (2nd-order Singly-Diagonal Implicit Runge-Kutta) [Alexander 1977], we solve two nonlinear systems to advance the state from step k to $k+1$:

$$\mathbf{M}\mathbf{v}^{(k+\alpha)} = \mathbf{M}\mathbf{v}^{(k)} + \alpha h\mathbf{f}^{(k+\alpha)} \tag{9a}$$

$$\mathbf{x}^{(k+\alpha)} = \mathbf{x}^{(k)} + \alpha h\mathbf{v}^{(k+\alpha)}, \tag{9b}$$

and

$$\mathbf{M}\mathbf{v}^{(k+1)} = \mathbf{M}\mathbf{v}^{(k)} + (1-\alpha)h\mathbf{f}^{(k+\alpha)} + \alpha h\mathbf{f}^{(k+1)} \tag{10a}$$

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + (1-\alpha)h\mathbf{v}^{(k+\alpha)} + \alpha h\mathbf{v}^{(k+1)}, \tag{10b}$$

where $\alpha = (2 - \sqrt{2})/2$. These two nonlinear systems are solved sequentially: first for $\mathbf{x}^{(k+\alpha)}$ and then for $\mathbf{x}^{(k+1)}$. (The velocities can be computed from the positions using Eqs. 9b and 10b.) Using the same process described in §1.1, the Newton search direction for the first nonlinear system becomes $\Delta\mathbf{x}_i = -\mathbf{H}_i^{-1}\mathbf{g}_i$, with

$$\begin{aligned} \mathbf{g}_i &= \mathbf{M}\left(\mathbf{x}_i^{(k+\alpha)} - \mathbf{x}^{(k)} - \alpha h \mathbf{v}^{(k)}\right) - (\alpha h)^2 \mathbf{f}_i^{(k+\alpha)} \\ \mathbf{H}_i &= \mathbf{M} - \alpha h \mathbf{D}_i^{(k+\alpha)} - (\alpha h)^2 \mathbf{K}_i^{(k+\alpha)}. \end{aligned} \tag{11}$$

Similarly, for the second nonlinear system, we have

$$\begin{aligned} \mathbf{g}_i &= \mathbf{M}\left(\mathbf{x}_i^{(k+1)} - \mathbf{x}^{(k)} - \beta h \mathbf{v}^{(k)} - \gamma h \mathbf{v}^{(k+\alpha)}\right) - (\alpha h)^2 \mathbf{f}_i^{(k+1)} \\ \mathbf{H}_i &= \mathbf{M} - \alpha h \mathbf{D}_i^{(k+1)} - (\alpha h)^2 \mathbf{K}_i^{(k+1)}, \end{aligned} \tag{12}$$

where $\beta = 2\alpha - 1$ and $\gamma = 2 - 2\alpha$.

2 ITERATION PLOTS

We list here the detailed iteration plots of the simulations. Each figure represents a test scene. For example, the rows of Fig. 1 correspond to the Young's modulus that was varied for the Bar scene. In each row, the left plot is the ND iterations, the middle plot is the QLF iterations, and the right plot is the QLB iterations. In all tests, the nonlinear solvers were run to convergence with a tolerance of 1e-6 for absolute or relative residual.

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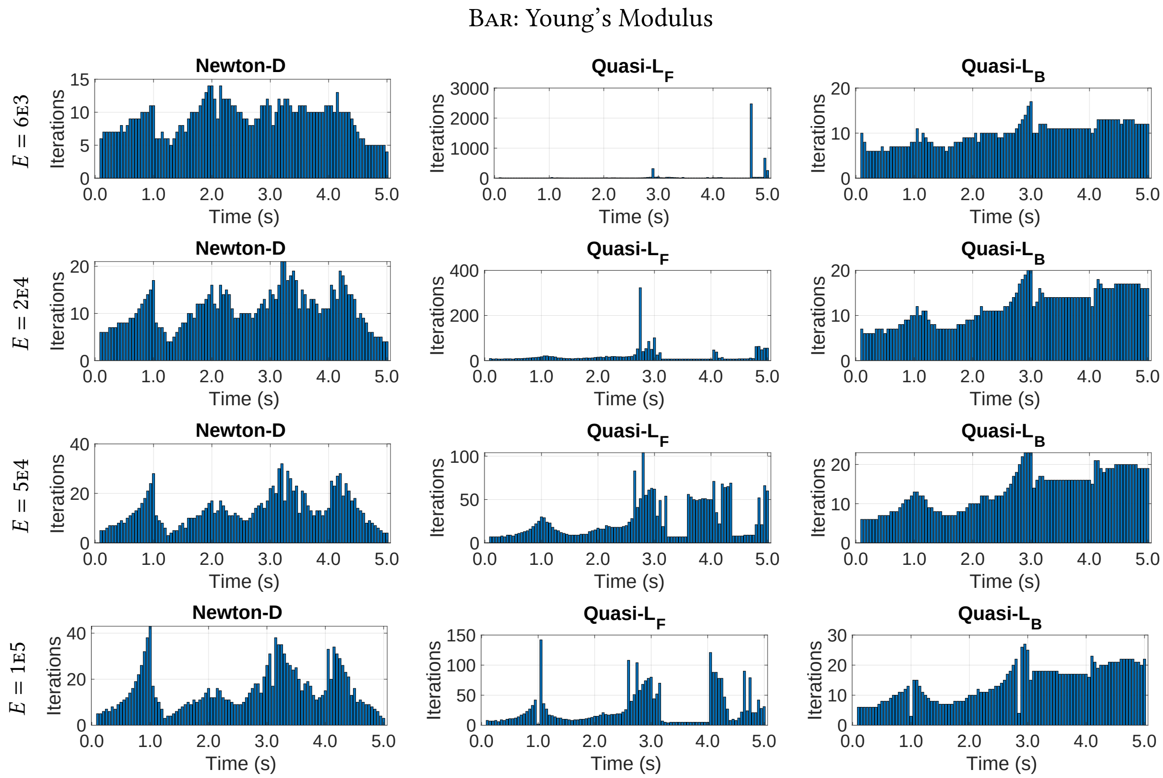

Fig. 1. Nonlinear iteration counts for the Bar scene with different Young's moduli. (Top) $E = 6\text{E}3$. (Middle-top) $E = 2\text{E}4$ [default]. (Middle-bottom) $E = 5\text{E}4$. (Bottom) $E = 1\text{E}5$.

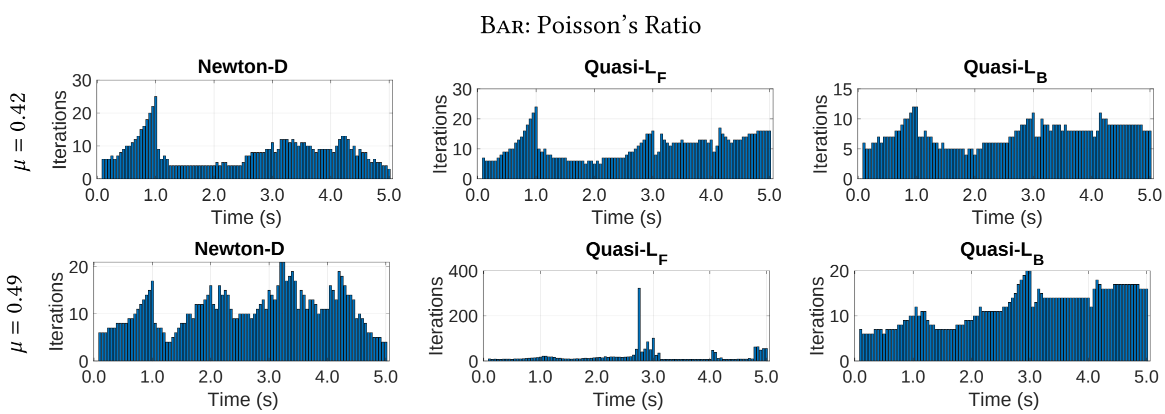

Fig. 2. Nonlinear iteration counts for the Bar scene with different Poisson's ratios. (Top) $\mu = 0.42$. (Bottom) $\mu = 0.49$ [default].

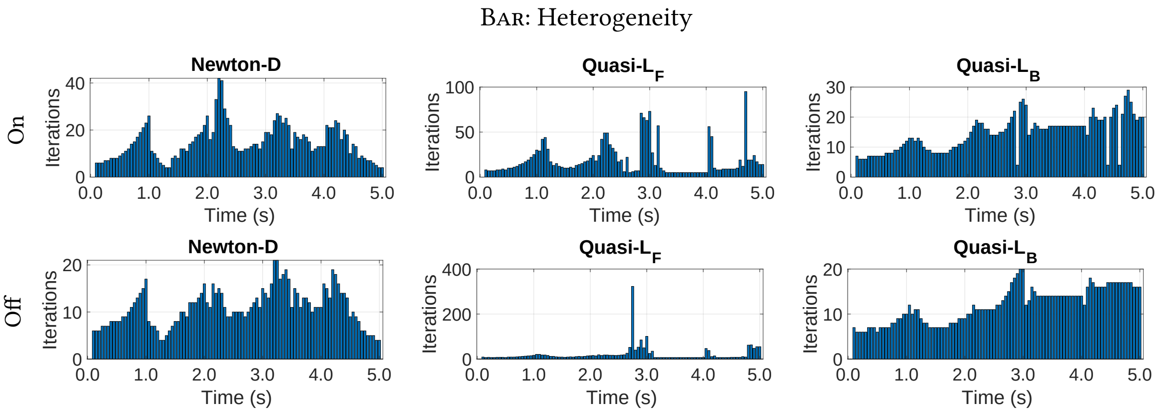

Fig. 3. Nonlinear iteration counts for the BAR scene with heterogeneity. (Top) with heterogeneity. (Bottom) without heterogeneity [default].

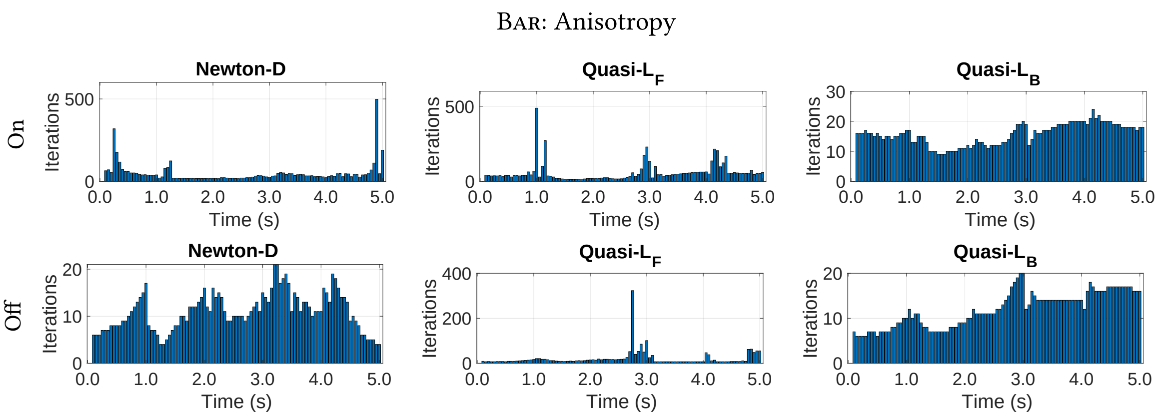

Fig. 4. Nonlinear iteration counts for the BAR scene with anisotropy. (Top) with anisotropy. (Bottom) without anisotropy [default].

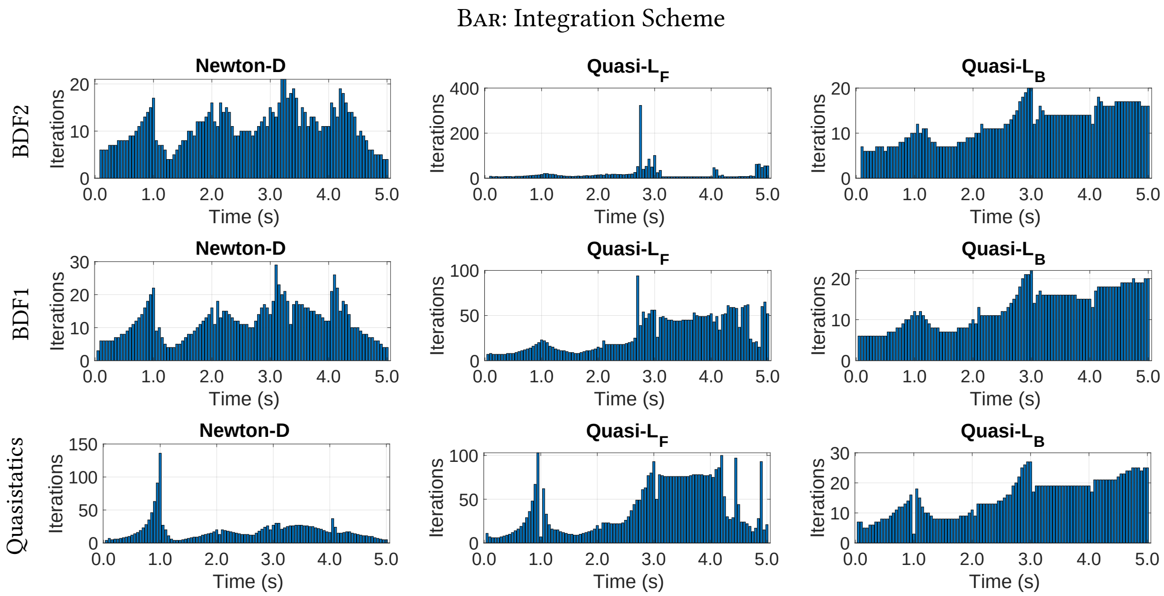

Fig. 5. Nonlinear iteration counts for the Bar scene with different integration schemes. (Top) BDF2 [default]. (Middle) BDF1. (Bottom) Quasistatics.

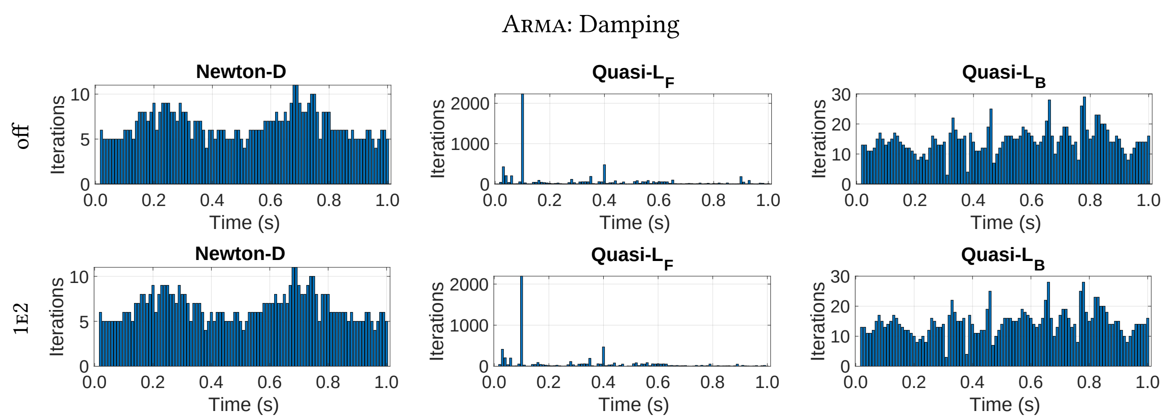

Fig. 6. Nonlinear iteration counts for the Arma scene with different damping coefficients. (Top) damping = 0 [default]. (Bottom) damping = 1e2.

ARMA: Material

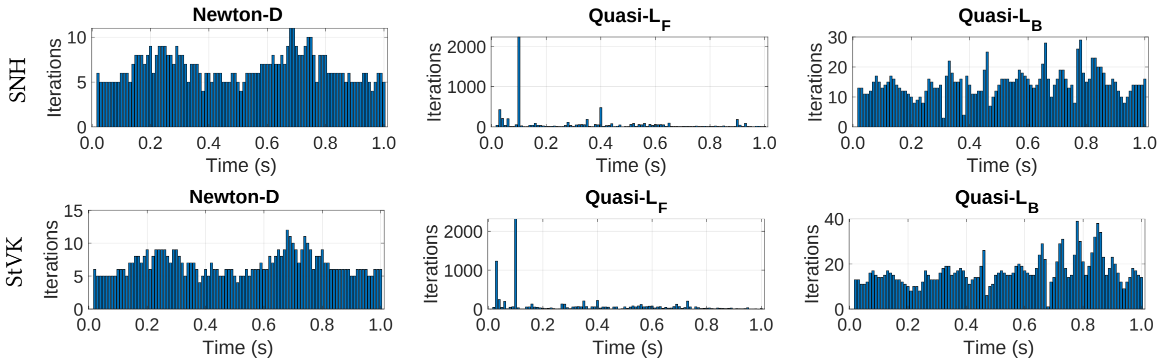

Fig. 7. Nonlinear iteration counts for the ARMA scene with different materials. (Top) SNH [default]. (Bottom) StVK.

ARMA: Time Step

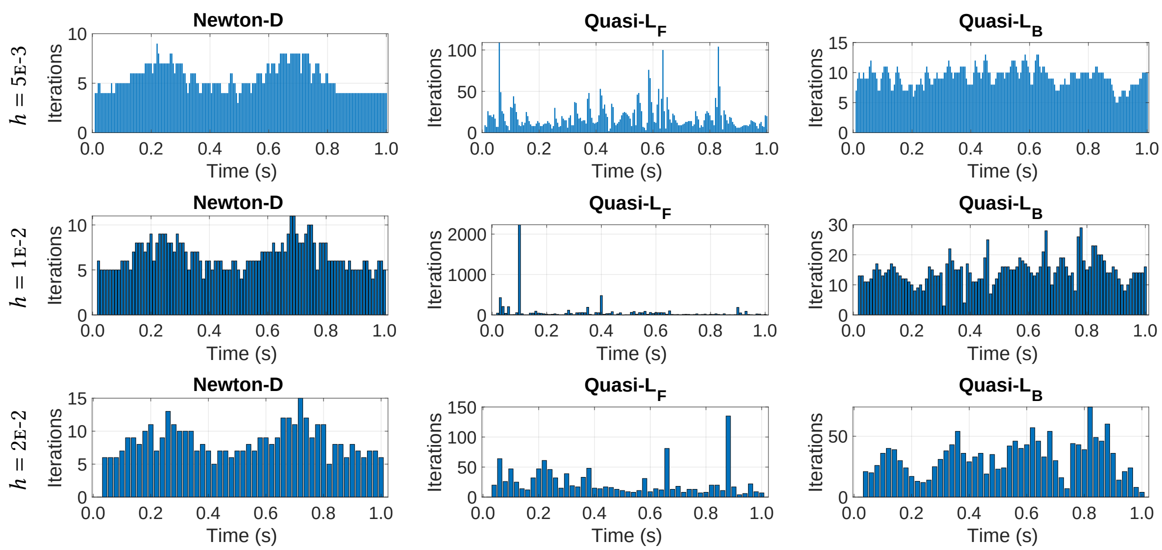

Fig. 8. Nonlinear iteration counts for the ARMA scene with different time steps. (Top) h = 5E-3. (Middle) h = 1E-2 [default]. (Bottom) h = 2E-2.

BUNNY

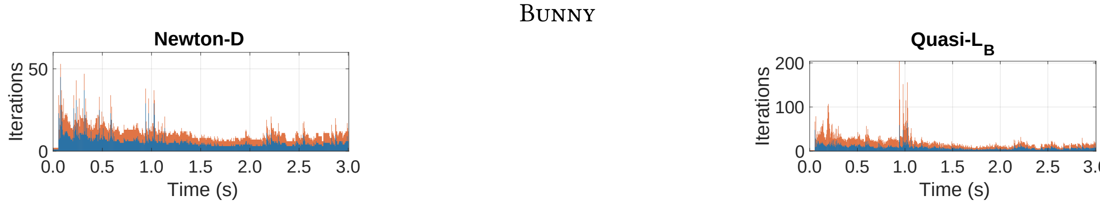

Fig. 9. Nonlinear iteration counts for the BUNNY scene. QLF did not converge. Blue is the first SDIRK2 solve, and red is the second.

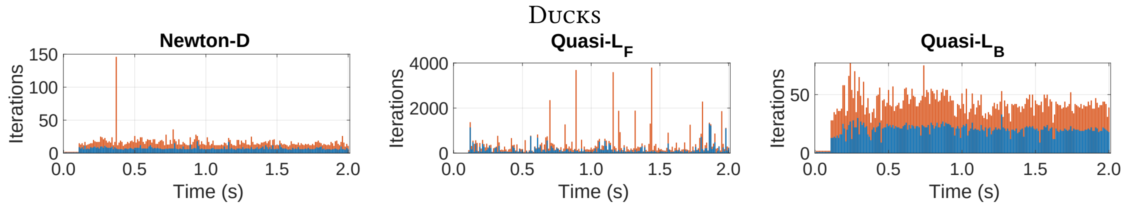

Fig. 10. Nonlinear iteration counts for the Ducks scene. Blue is the first SDIRK2 solve, and red is the second.