

Numerical Reduced Order Modeling for Wave Equations in Heterogeneous Media

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Support: **NSF** and **DOE**.

Maxwell's equations for a dispersive medium:

$$\begin{aligned}\frac{\partial}{\partial t}(E + \mathcal{K}_e * E) &= \frac{1}{\epsilon_0} \nabla \times H \\ \frac{\partial}{\partial t}(H + \mathcal{K}_m * H) &= -\frac{1}{\mu_0} \nabla \times E\end{aligned}$$

Typically describe the convolution kernels via their Laplace transform - for isotropic problems they will be scalar but in anisotropic cases they will be matrices. In all the examples we consider the convolutions are “lower order” terms in that:

$$\lim_{s \rightarrow \infty} \hat{\mathcal{K}}_{e,m} = 0.$$

We believe that this condition combined with the condition that $\hat{\mathcal{K}}$ is analytic in $\Re s > 0$ implies the well-posedness of the Cauchy problem and finite propagation speed. (Proof? Hille-Yosida + Paley-Wiener?)

These are multiscale models in that the convolutional terms model the interaction of the complex medium with the waves.

Dispersion relation $s = -i\omega$, isotropic case:

$$\omega^2(1 + \hat{\mathcal{K}}_e(-i\omega))(1 + \hat{\mathcal{K}}_m(-i\omega)) = |k|^2$$

Group velocity - convenient formula from, “On the analysis of perfectly matched layers for a class of dispersive media and applications to negative index metamaterials”, Bécache, Joly and Violes, Math. Comp. 2018.

$$V_g = c_0 \frac{2\sqrt{(1 + \hat{\mathcal{K}}_e)(1 + \hat{\mathcal{K}}_m)}}{\left((1 + \hat{\mathcal{K}}_e) \frac{d}{d\omega} \left(\omega(1 + \hat{\mathcal{K}}_m) \right) (1 + \hat{\mathcal{K}}_m) \frac{d}{d\omega} \left(\omega(1 + \hat{\mathcal{K}}_e) \right) \right)} \frac{k}{|k|}.$$

One of many interesting phenomena in metamaterials is the possibility of reverse modes: $V_g \cdot V_p < 0$, where V_p is the phase velocity - here is an illustration with a simple Drude model and TE modes:

$$\hat{\mathcal{K}}_e = \frac{\omega_e^2}{s^2}, \quad \hat{\mathcal{K}}_m = \frac{\omega_m^2}{s^2},$$

We force it at 3 different frequencies - one with phase and group velocity aligned, one in the band gap, and one with reverse modes.

As in the Drude model, there are many instances where the convolution can be approximated to the desired accuracy by a sum of localizable convolutions - that is we can take $\hat{\mathcal{K}}_{e,m}$ to be rational functions of s . More directly this will be true if $\hat{\mathcal{K}}_{e,m}$ can be approximated uniformly by rational functions on an appropriate inversion contour:

$$\hat{\mathcal{K}}_e \approx \sum_{j=1}^{n_e} \frac{\alpha_{e,j}s + \beta_{e_j}}{(s + \gamma_{e,j})^2 + \eta_{e,j}^2},$$

$$\hat{\mathcal{K}}_m \approx \sum_{j=1}^{n_m} \frac{\alpha_{m,j}s + \beta_{m_j}}{(s + \gamma_{m,j})^2 + \eta_{m,j}^2}.$$

In the time domain this corresponds to approximating $\mathcal{K}_{e,m}$ by sums of exponential/trigonometric functions. Such approximations were used, for example, to evaluate exact radiation boundary conditions by Alpert, Greengard and H, (SINUM 2000). A general algorithm for their computation is given in Xu and Jiang, (J. Sci. Comput. 2013). The idea is to use a linearized rational least squares algorithm and slowly add poles.

More generally one can construct such approximations after removing a small nonsmooth part of the convolution near $t = 0$ - corresponds to nonsmooth behavior of $\hat{\mathcal{K}}$ for large s - we will mention this later on when considering dispersion relations involving fractional derivatives. Another very general approach is based on piecewise (in t) exponential/trigonometric approximations using quadrature on appropriate contours; see Lubich and Schädle (SISC 2002); see also Trefethen, Weideman and Schmeizer (BIT 2006).

Interpolatory methods (data based - now called machine learning!) - e.g. the AAA algorithm (Nakatsukasa, Sète, Trefethen 2018), rational Krylov (Güttel - rktoolbox), AAK variant (Damle, Beylkin, Haut and Monzon 2018)

Note that if $\alpha = \gamma = 0$ one obtains the generalized Lorentz models considered by Bécache et al. In any case we can introduce auxiliary variables so that the model becomes a symmetrizable hyperbolic system with a zero order perturbation:

$$\begin{aligned}
\frac{\partial E}{\partial t} &= \frac{1}{\epsilon_0} \nabla \times H - \sum_{j=1}^{n_e} \alpha_{e,j} E - \gamma_{e,j} P_j + Q_j \\
\frac{\partial H}{\partial t} &= -\frac{1}{\mu_0} \nabla \times E - \sum_{j=1}^{n_m} \alpha_{m,j} H - \gamma_{m,j} R_j + V_j \\
\frac{\partial P_j}{\partial t} &= \alpha_{e,j} E - \gamma_{e,j} P_j + Q_j \\
\frac{\partial Q_j}{\partial t} &= \eta_{e,j} E - \beta_{e,j}^2 P_j - \gamma_{e,j} Q_j \\
\frac{\partial R_j}{\partial t} &= \alpha_{m,j} H - \gamma_{m,j} R_j + V_j \\
\frac{\partial V_j}{\partial t} &= \eta_{m,j} H - \beta_{m,j}^2 R_j - \gamma_{m,j} V_j
\end{aligned}$$

Succinctly with scaling the system can be put in the form:

$$\frac{\partial W}{\partial t} = A_1 \frac{\partial W}{\partial x} + A_2 \frac{\partial W}{\partial y} + A_3 \frac{\partial W}{\partial z} + SW,$$

where $A_j = A_j^T$ and in some cases with scaling $S + S^T \leq 0$. (For the Lorentz case $S + S^T = 0$ - see Bécache et al). (Stability analysis for S with nonpositive eigenvalues but not symmetrizable is more involved - symmetrizers in frequency space.)

We conclude that the system:

- Leads to a well-posed Cauchy problem.
- Has the same domain of dependence as the nondispersive Maxwell system.
- Is well posed under the same boundary conditions as the nondispersive Maxwell system.

Given these facts stability proofs for many numerical methods are directly generalizable to these models. For example Yang, Huang and Li (J. Sci. Comput. 2016) develop methods based on edge elements. For example we can use standard central or upwind DG schemes, but also other energy stable methods such as dissipative or conservative Hermite methods.

For a DG scheme we use the fact that the fluxes are unchanged, so we have:

$$\int_{\Omega_j} \Phi^T \frac{\partial W}{\partial t} - \Phi^T A_1 \frac{\partial W}{\partial x} - \Phi^T A_2 \frac{\partial W}{\partial y} - \Phi^T A_3 \frac{\partial W}{\partial z} - \Phi^T S W - \int_{\partial\Omega_j} \Phi^T (n \cdot A)(W - W^*) = 0.$$

Choosing the fluxes exactly as for the nondispersive Maxwell system, as they are the only terms that appear in $n \cdot A$, and choosing the test function $\Phi = W$ we have

$$\frac{d}{dt} \sum_j \int_{\Omega_j} |W|^2 \leq \sum_j \int_{\Omega_j} W^T (S + S^T) W,$$

immediately yielding stability. If we further assume $S + S^T \leq 0$ we conclude that the L^2 norm is uniformly bounded in time.

There are dispersive models which can't be accurately represented by rational functions due to irregularity of the convolution kernel for short times (or its transform for large s). An example is given by Havriliak-Negami dielectric model which involves fractional derivatives: for $0 < \alpha \leq 1$, $0 < \beta \leq 1$

$$\hat{\mathcal{K}}_e = \frac{\eta}{(1 + (s\tau)^\alpha)^\beta}.$$

Incorporation of this model into the Yee scheme is achieved in Causley, Petropoulos and Jiang (JCP 2011). For small t they directly treat the convolution over the current time step using an expansion of \mathcal{K}_e :

$$\mathcal{K}_e(t) \approx \frac{\eta}{\tau} \sum_k c_k(\alpha, \beta) \left(\frac{t}{\tau}\right)^{\alpha(k+\beta)-1}.$$

They then build a modification of the Yee scheme to account for the local behavior. For the history, that is the convolution past Δt , they use a rational approximation as above computed via quadrature applied to integral representations of the kernel.

Recently Baffet and Hesthaven have used the arguments in Alpert, Greengard, H. to directly construct approximations to time fractional derivative operators Δt away from the current time and manage to construct a scheme where the pole locations are independent of Δt to allow high order adaptive time stepping based on Adams methods. (Math. Comp., J. Sci. Comput. 2017).

All of this assumes that $\mathcal{K}_{e,m}$ is known. In many cases this may not be true - as shown, e.g., in work by Bouchitté a first approximation can be obtained using homogenization theory, but formally at least these formulas require a very large scale separation.

This leads to the question of whether a numerical approach could be useful - numerical multiscale methods. (Review by Abdulle and Henning 2018) Much work leverages ideas from elliptic problems - doesn't really take advantage of the fundamental feature of hyperbolic pdes which is local domain-of-dependence.

The most famous method is the so-called Heterogeneous Multiscale Method (HMM). (e.g. E and Engquist, Multiscale Methods in Science and Engineering, 2009).

The basic idea of the HMM framework is to:

- Assume a macroscopic model exists (in our case the dispersive Maxwell system)
- Introduce a macro numerical method appropriate to the model
- Solve the full microscopic model in microscopic neighborhoods of quadrature/flux nodes of the macroscopic discretization and average over space-time to provide the missing quadrature/flux data.

An issue in applying HMM to wave problems is that the local solutions oscillate in time rather than relax. There are some recent papers on the scalar wave equation.

Arjmond and Runborg, Mult. Mod. Sim. 2014 Here they study the ill-posed macro model:

$$\frac{\partial^2 u}{\partial t^2} = \alpha \frac{\partial^2 u}{\partial x^2} + \epsilon^2 \beta \frac{\partial^4 u}{\partial x^4}$$

They use the wave equation as the microscopic model with specially prepared initial data and averaging operators and prove that the flux in their discretization is correct with a small error.

Abdulle, Grote and Stohrer, Comptes Rendu Math. 2013 Here they study the well-posed macro model:

$$\frac{\partial^2 u}{\partial t^2} = \alpha \frac{\partial^2 u}{\partial x^2} + \epsilon^2 \frac{\beta}{\alpha} \frac{\partial^4 u}{\partial x^2 \partial t^2}$$

They solve the Neumann problem in the microscopic level and use the solution both in the quadrature for the mass matrix and the stiffness matrix:

$$\begin{aligned} \frac{\partial^2}{\partial t^2} ((u_H, v_H) + (u_H, v_H)_M) + B_H(u_H, v_H) &= (f, v_H) \\ \sum_{T_H} \sum_j \frac{w_j}{|K_\delta|} \int_{K_\delta} a_\epsilon(x) \nabla v_h \cdot \nabla w_h &= B_H(v_H, w_H) \\ \sum_{T_H} \sum_j \frac{w_j}{|K_\delta|} \int_{K_\delta} (v_h - v_{H,lin}) \cdot (w_h - w_{H,lin}) &= (v_H, w_H)_M \\ \int_{K_\delta} a_\epsilon(x) \nabla (v_h - v_{H,lin}) \cdot \nabla z_h &= 0. \end{aligned}$$

Question: How can we apply this method to Maxwell's equations where the macroscopic model is the dispersive system we've been talking about?

Other ideas I am interested in:

- Skeletonized approximations based on local radiation conditions - first order system extension of the multiscale reduced-order model for second order wave equations by Druskin, Mamanov and Zaslavsky (MMS 2017). (Not yet implemented.)
- Approximation of the solution operator on staggered grids. (Suboptimal implementation in 1d).

Simple 1d model:

$$\begin{aligned}\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} + q(x/\epsilon)v &= 0 \\ \frac{\partial v}{\partial t} - \frac{\partial v}{\partial x} - q(x/\epsilon)u &= 0\end{aligned}$$

Note that the L^2 -norm of the solution is conserved (modulo boundary contributions). Fine scale discretization based on central or upwind DG methods is straightforward.

Idea behind the skeletonized approximations - should be particularly useful for problems with small inclusions as in some metamaterials.

Let $[x_L, x_R]$ be a coarse element. Inspired by a typical DG formulation consider the incoming variables as known:

$$u(x_L, t) = U_L(t), \quad v(x_R, t) = V_R(t).$$

Then there is a unique causal solution which can be used to express the outgoing waves:

$$\begin{aligned} v(x_L, t) &= K_{LL} * U_L(t) + K_{LR} * V_R(t) \\ u(x_R, t) &= K_{RL} * U_L(t) + K_{RR} * V_R(t). \end{aligned}$$

The unknowns in the skeletonized method, $u_j(t)$, $v_j(t)$ are simply the fields at the element boundaries. Again assuming the kernels are known we have the convolution-difference equations:

$$\begin{aligned} u_j(t) &= K_{RL,j-1/2} * u_{j-1}(t) + K_{RR,j-1/2} * v_j(t) \\ v_j(t) &= K_{LL,j+1/2} * u_j(t) + K_{LR,j+1/2} * v_{j+1}(t). \end{aligned}$$

The problem is to compute approximations to the convolution kernels using localized fine grid computations. Here it is natural to first apply a Laplace transformation in t :

$$\begin{aligned} s\hat{u} + \frac{\partial \hat{u}}{\partial x} + q(x/\epsilon)\hat{v} &= 0 \\ s\hat{v} - \frac{\partial \hat{v}}{\partial x} - q(x/\epsilon)\hat{u} &= 0 \end{aligned}$$

For fixed s we can solve, for example, using a well-resolved upwind DG discretization - e.g. on macro cell $j + 1/2$:

$$\begin{pmatrix} sI + D + L & Q \\ -Q & sI - D - L \end{pmatrix} \begin{pmatrix} \hat{u}^{j+1/2} \\ \hat{v}^{j+1/2} \end{pmatrix} = \begin{pmatrix} L & 0 \\ 0 & -L \end{pmatrix} \begin{pmatrix} \hat{u}_j \\ \hat{v}_{j+1} \end{pmatrix}.$$

The solution of this system yield an approximation - high-degree rational function of s - to the Laplace transforms of the kernels in the convolution-difference equations:

$$\begin{aligned} \hat{u}_{j+1} &= \hat{K}_{RL,j+1/2}^h(s)\hat{u}_j + \hat{K}_{RR,j+1/2}^h\hat{v}_{j+1} \\ \hat{v}_j &= \hat{K}_{LL,j+1/2}^h(s)\hat{u}_j + \hat{K}_{LR,j+1/2}^h\hat{v}_{j+1}. \end{aligned}$$

As they stand the degree of these rational functions scales poorly:

$$\text{degree} \propto h^{-1} \sim \epsilon^{-1}$$

To produce a reduced order model one must use one of the various rational compression methods mentioned above, maintaining stability and causality.

In multiple dimensions the procedure is the same once one introduces incoming and outgoing variables (upwind fluxes) on the element boundaries. However, compressing the convolution kernels is not enough since the boundary traces for the numerical scheme are given in the fine space. That is

$$u_j = \sum_{k=O(\epsilon^{1-d})} u_{j,k}$$

A typical control theory approach to this reduction is to use balanced truncation or balanced proper orthogonal decomposition - variant of proper orthogonal decomposition.

Druskin et al propose another approach. The second reduction (actually done first!) leads to reduced spatial bases on the skeleton.

The second method uses staggered coarse cells and domain-of-dependence considerations to derive localized evolution operators.

For example consider 2 neighboring coarse cells of width H :

$$[x_{j-1}, x_j] \cup [x_j, x_{j+1}].$$

Assuming a maximum wave speed of 1 as in the model problem and a large time step Δt satisfying the CFL condition:

$$\Delta t < \frac{H}{2}$$

the solution on the staggered cell $[x_{j-1/2}, x_{j+1/2}]$ at time $t + \Delta t$ depends only on the data in the two cells at time t .

$$\begin{pmatrix} u^j(t + \Delta t) \\ v^j(t + \Delta t) \end{pmatrix} = S_{j,j-1/2}(\Delta t) \begin{pmatrix} u^{j-1/2}(t) \\ v^{j-1/2}(t) \end{pmatrix} + S_{j,j+1/2}(\Delta t) \begin{pmatrix} u^{j+1/2}(t) \\ v^{j+1/2}(t) \end{pmatrix}.$$

Obviously these operators can be approximated by local fine grid computations. To get a viable reduced-order-method one can again use the balanced truncation - balanced POD construction to compute an effective reduced basis for the elements.

We have implemented this method, but with naive reduced bases - Legendre polynomials and L^2 projections.

My one numerical example!

Domain $[-1, 1] \times [0, 20]$ with periodic boundary conditions.

Potential $q = \sum_{k=1}^{150} a_k \sin k\pi x$, a_k uniformly distributed in $[-1, 1]$.

Initial Data $u = 1 + \cos(\pi t)$, $v = 0$.

Coarse Grid $H = 1/10$, $\Delta t = 1/40$.

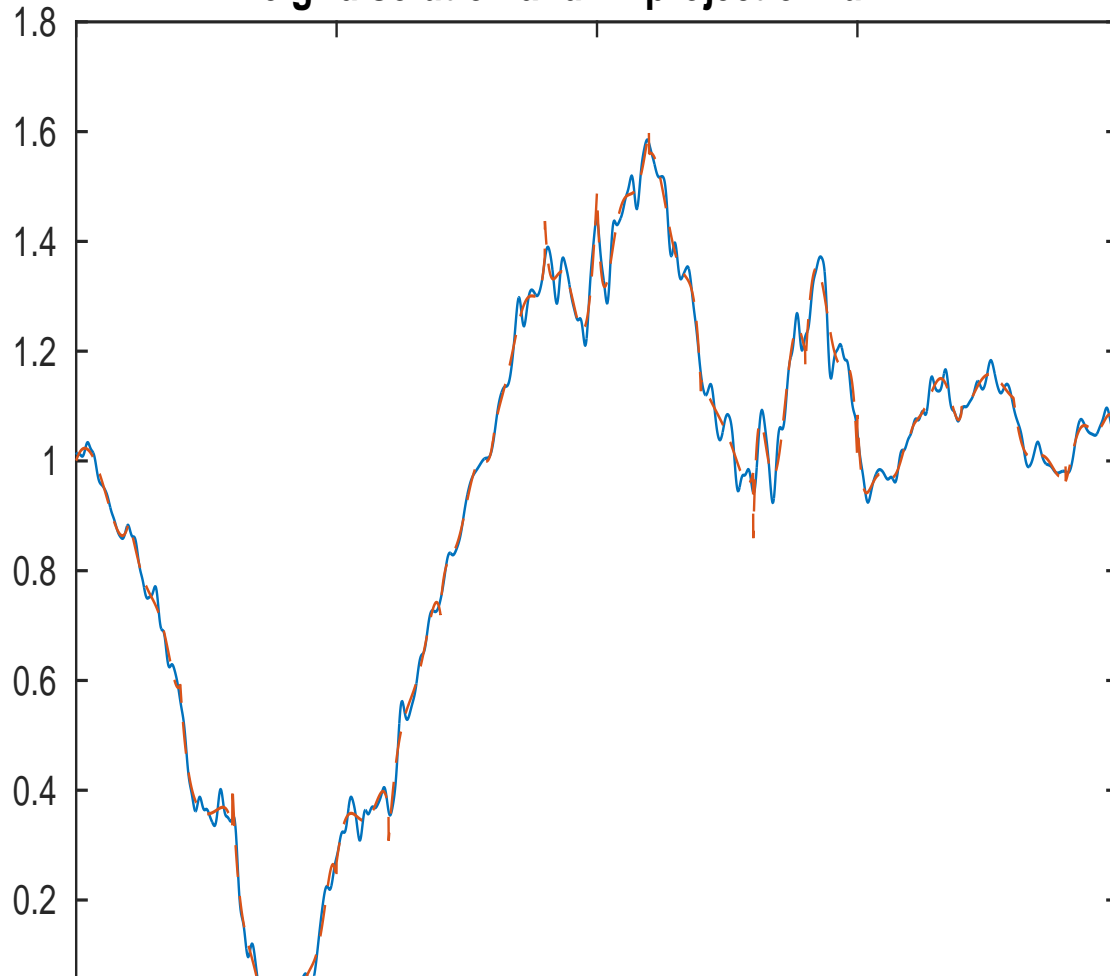
Fine Grid $h = 1/300$, $\delta t = 1/6000$.

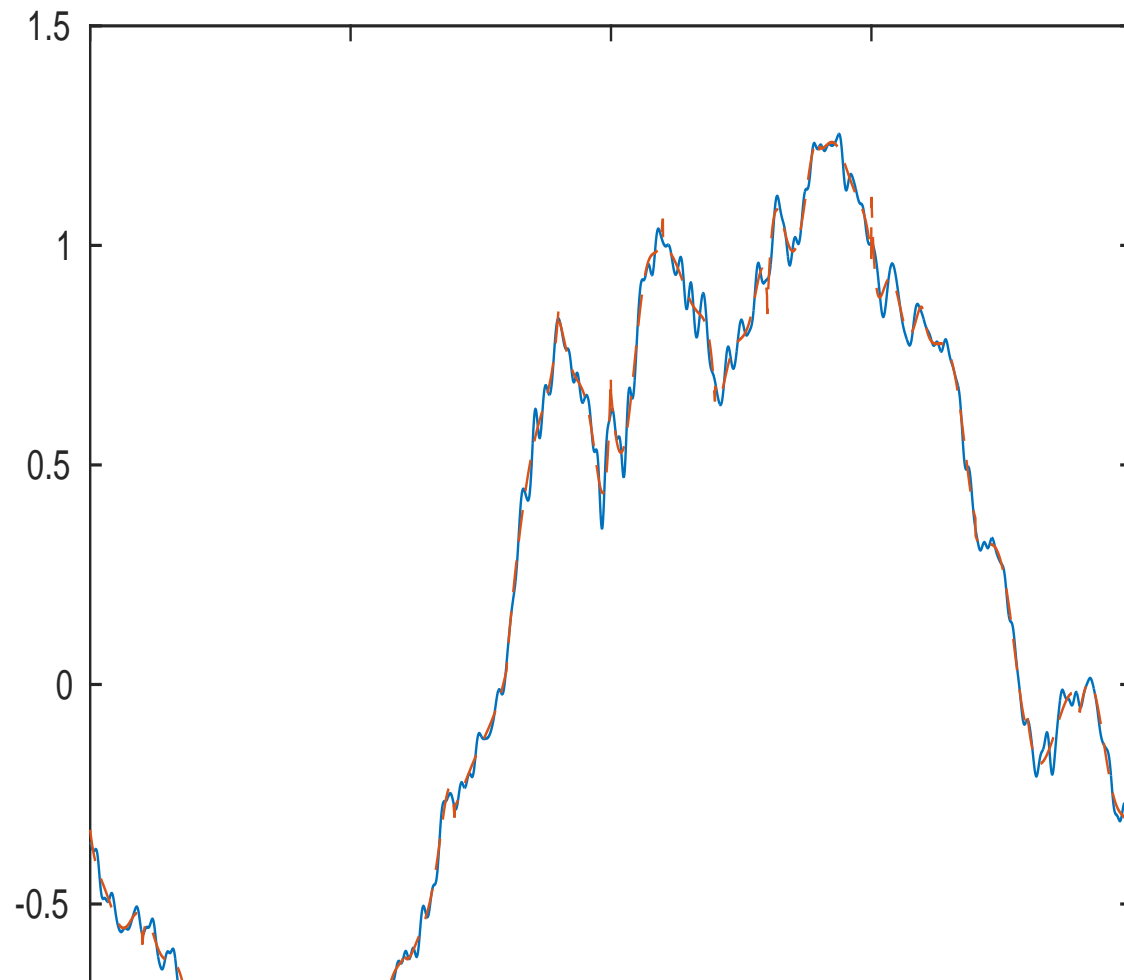
Fine Scale Method Upwind DG, degree 5 polynomials, RK4 in time.

Coarse Grid Projections Degree 5 polynomials

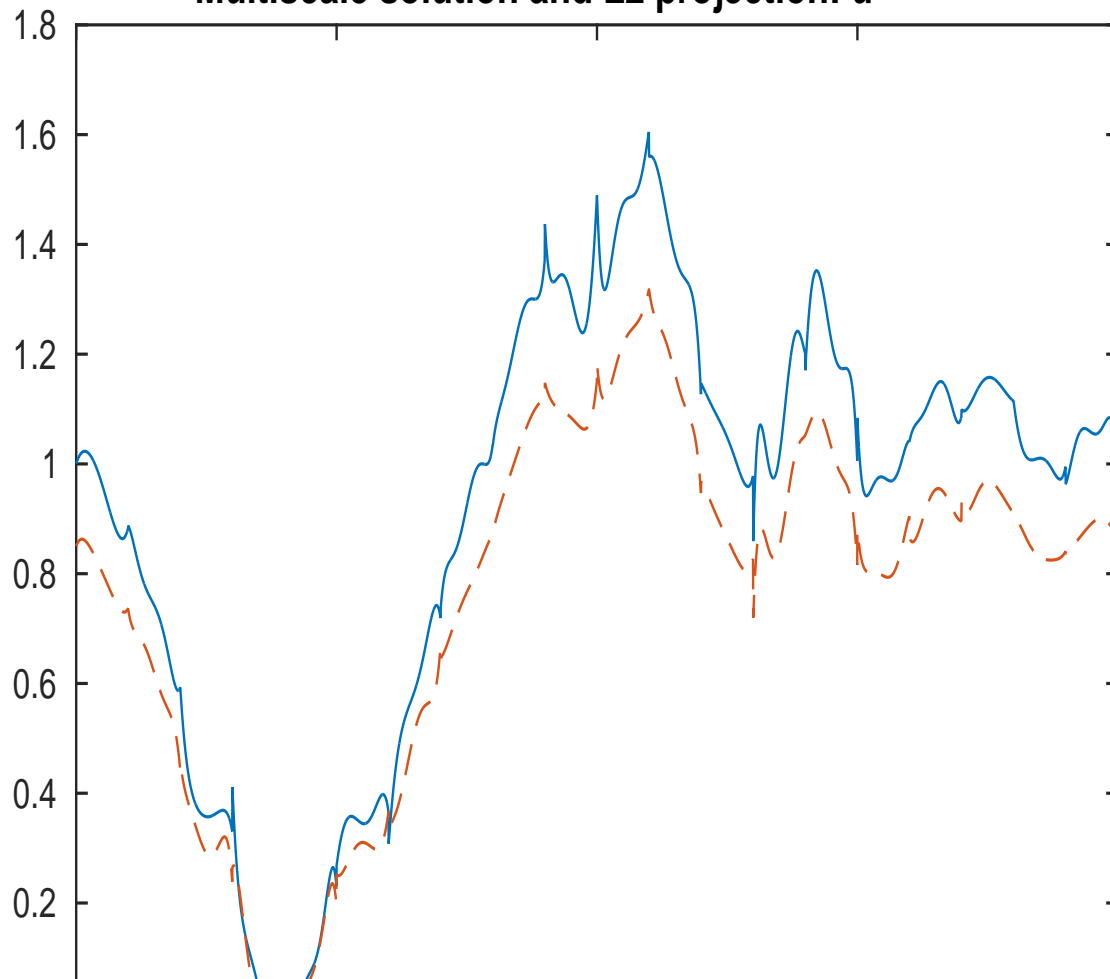
Results: some accuracy, but L^2 projections are a bit too dissipative. But the reduction in work would translate to a factor of more than 4×10^6 in $3 + 1$ dimensions!

Fine grid solution and L2 projection: u

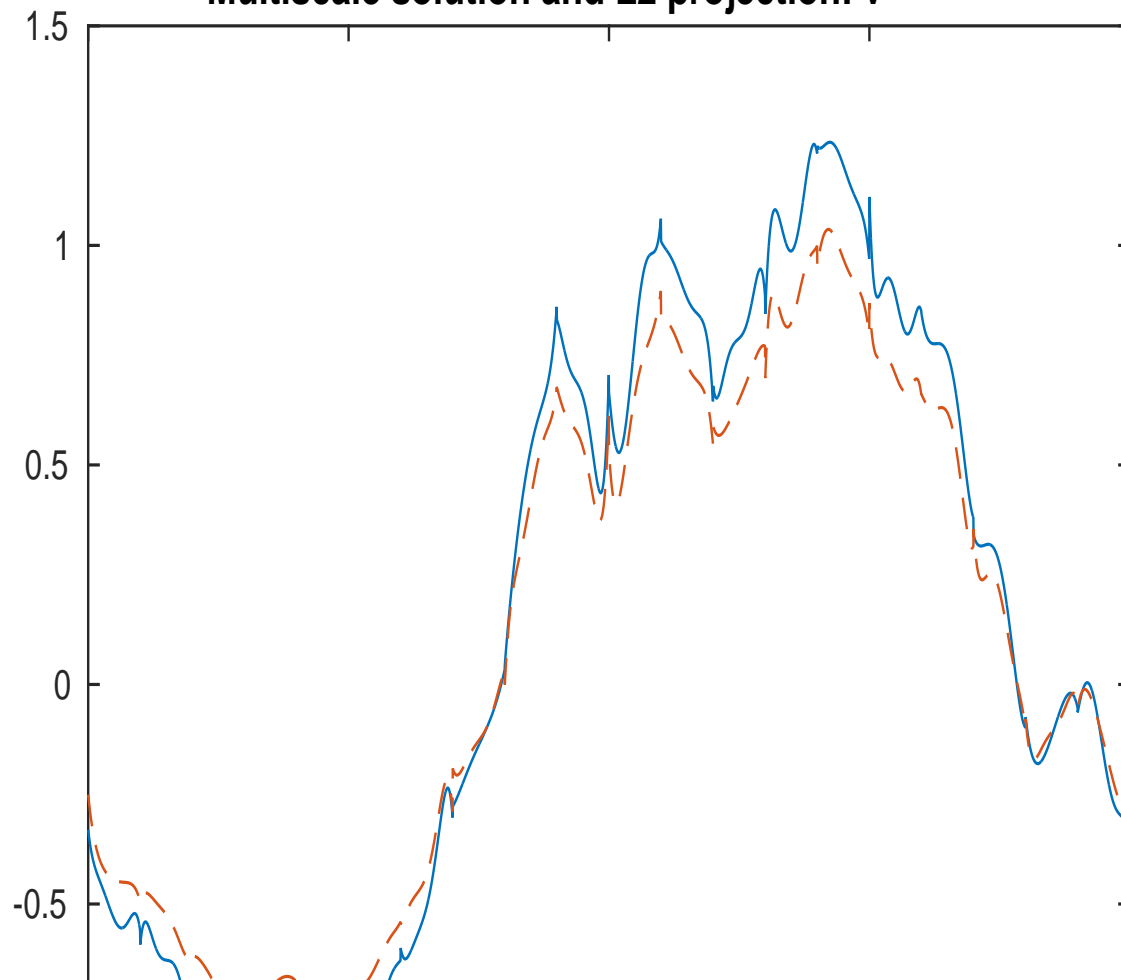




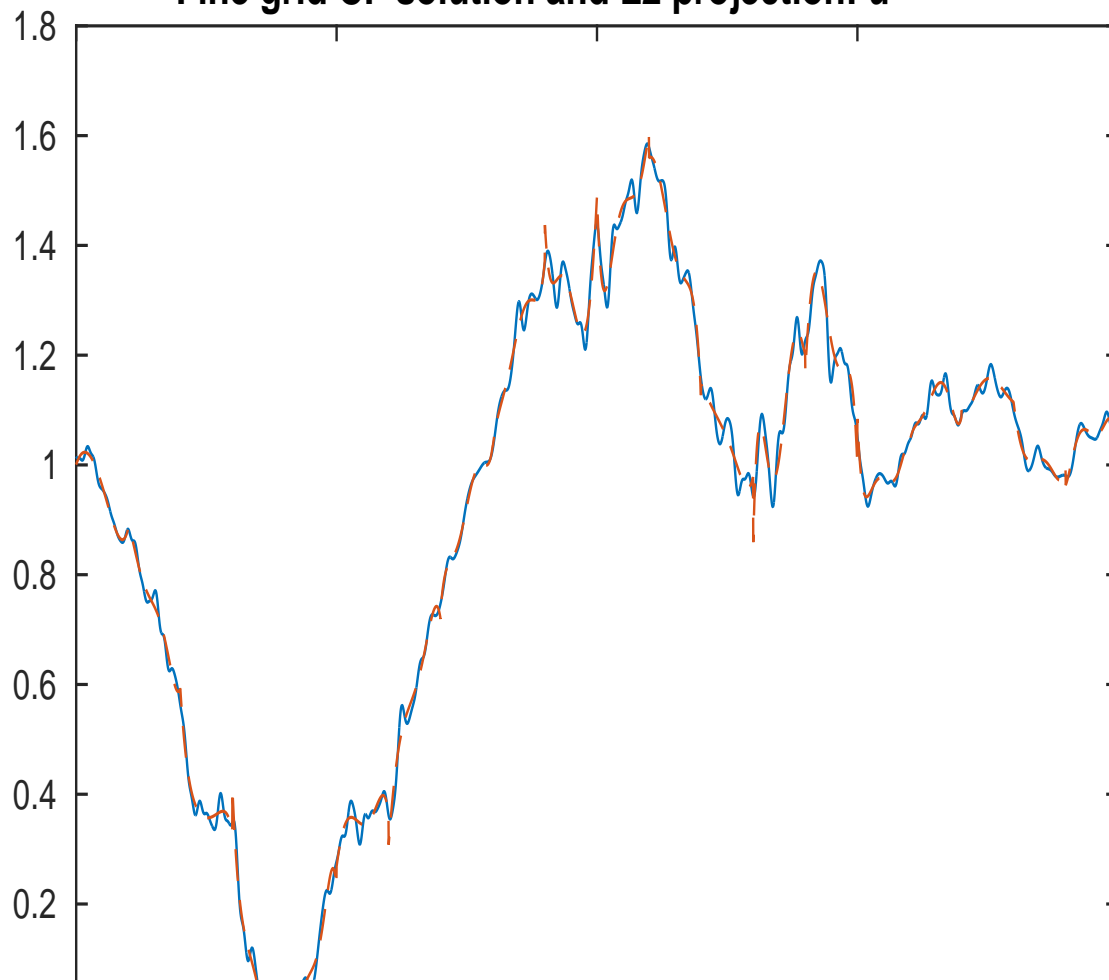
Multiscale solution and L2 projection: u



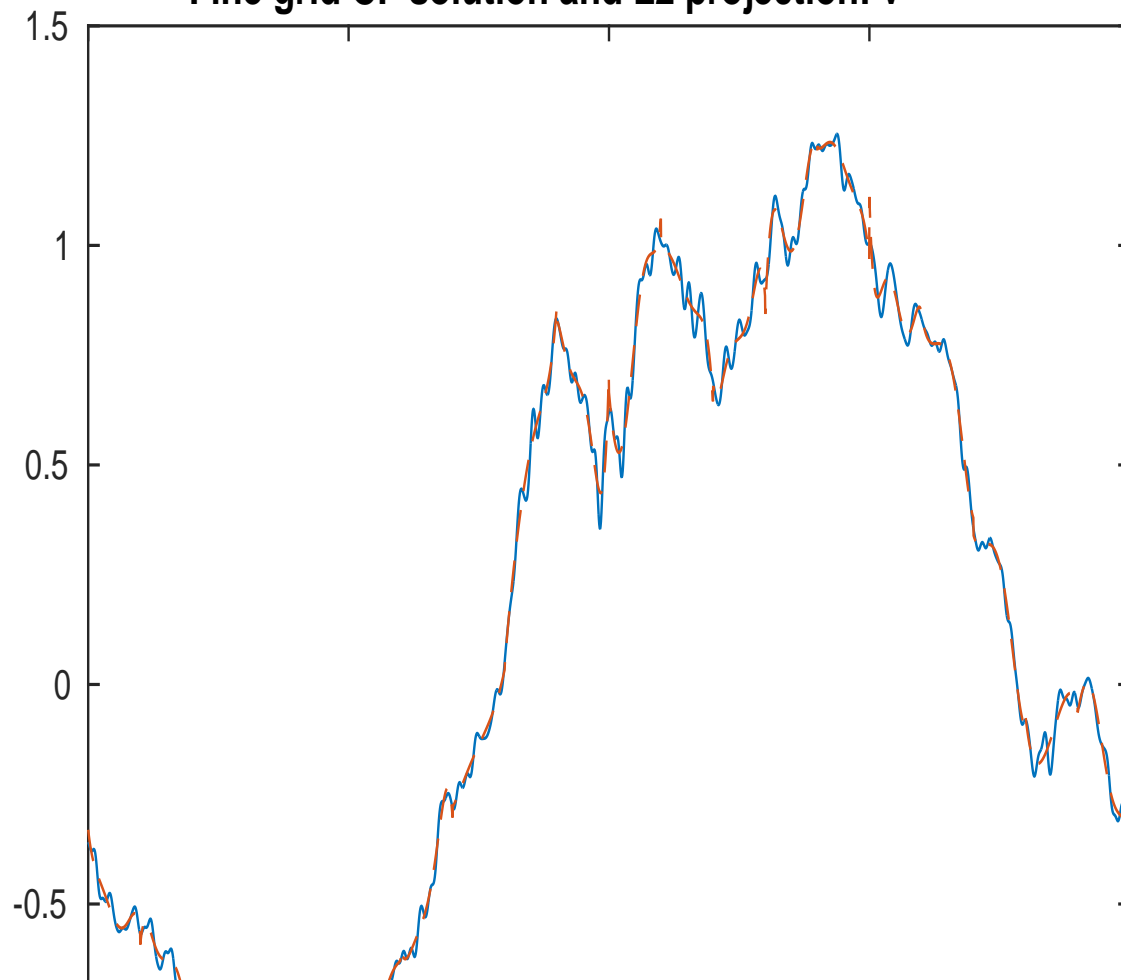
Multiscale solution and L2 projection: v



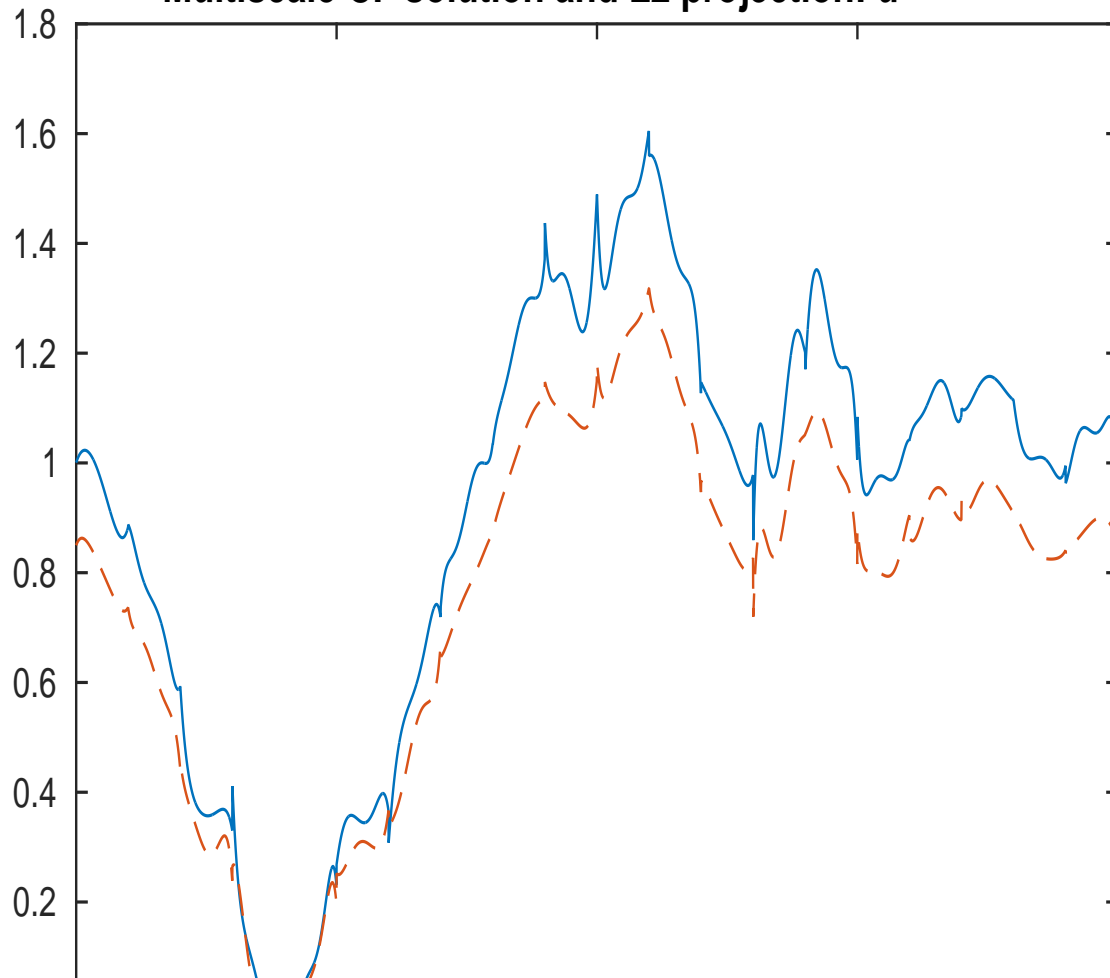
Fine grid CF solution and L2 projection: u



Fine grid CF solution and L2 projection: v



Multiscale CF solution and L2 projection: u



Multiscale CF solution and L2 projection: v

