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Synchronous and Asynchronous Time Integration for Multiscale Simulations Using Hybridized Finite Element Methods

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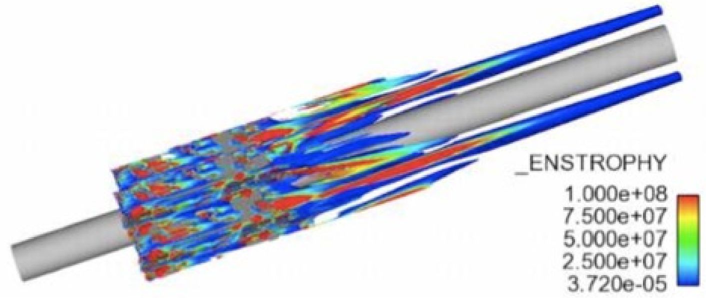
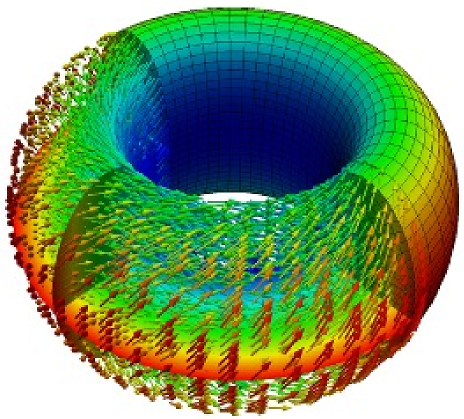
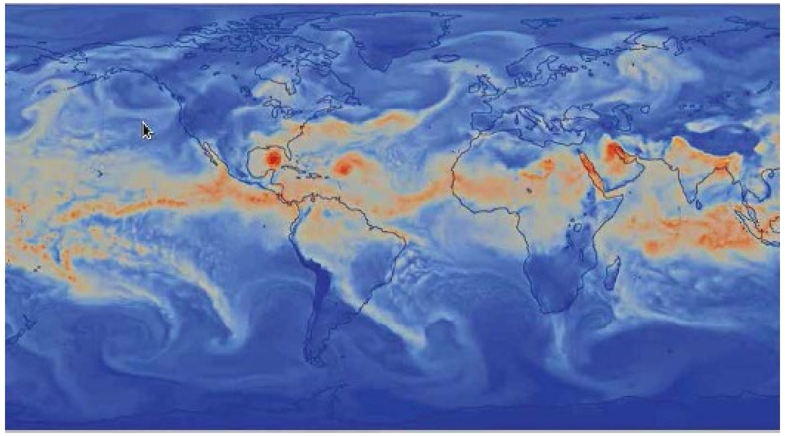
Introduction and Background

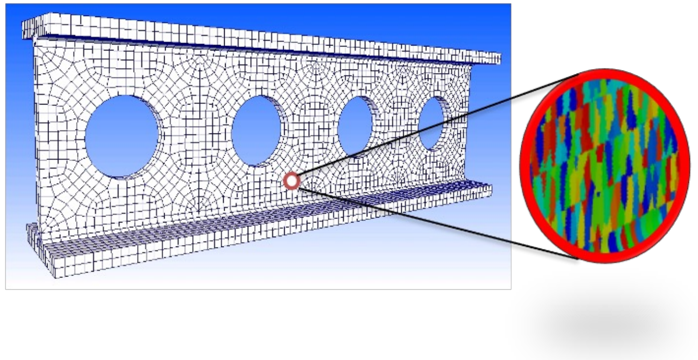
Motivation





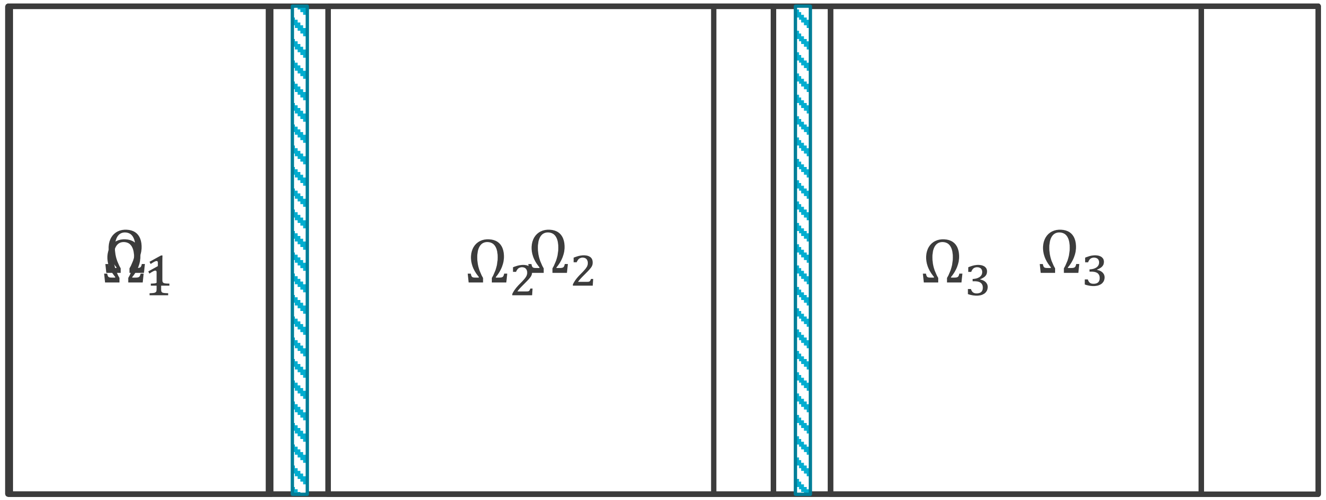
Many practical science/engineering problems are multiscale in both space and time





Hybridized finite element methods are well-suited for multiscale simulation

- Hybridized finite element (HFE) methods introduce additional unknowns along subdomain boundaries
- Subdomains interact solely through these unknowns
- Enables different discretizations, physics, numerical methods
- Can be interpreted as variational multiscale methods



Interest in alternative time integration schemes to bolster applicability of HFE methods

- Most HFE schemes are implicit
- Recent interest in explicit and implicit/explicit (IMEX) methods
  - E.g., Kronbichler (2015), Stanglmeier (2016), Samii (2019)
- Alternative time integration strategies could make HFE more attractive
- HFE framework offers flexibility (spatially and temporally)

Synchronous and Asynchronous Time Integrators

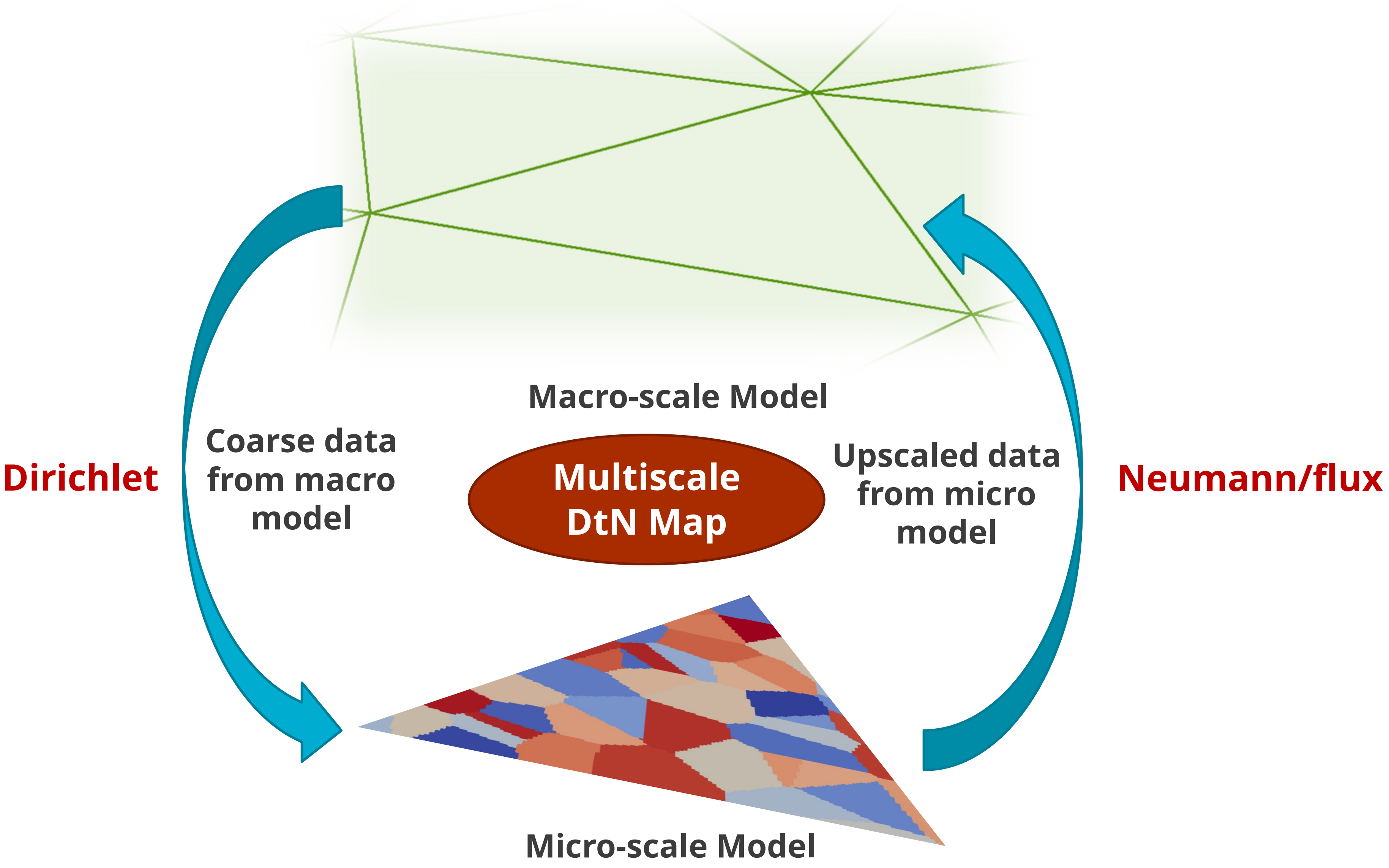
Concurrent multiscale framework leads to "macro-micro-macro" map

$$\frac{\partial u_c}{\partial t} = F_c(u_c, u_f)$$

$$\frac{\partial u_f}{\partial t} = F_f(u_c, u_f)$$

$$\frac{\partial u_c}{\partial t} = F_c(u_c, h(u_c))$$

MrHyDE Provides a General Framework for Concurrent Multiscale Methods



HFE methods produce coupled multiscale systems

1) $$\frac{\partial u}{\partial t} + \nabla \cdot F(u) = G(u), \qquad in\ \Omega \times (0,T]$$

Partitioning $$\Omega = \bigcup_{i=1}^{N} \Omega_i$$

Skeleton $$\mathcal{E} = \bigcup_{1 \le i \le j \le N} \partial\Omega_i \cap \partial\Omega_j$$

2) $$\begin{cases} \dfrac{\partial u_i}{\partial t} + \nabla \cdot F(u_i) = G(u_i), \qquad in\ \Omega_i \times (0,T] \\ u_i = \lambda, \qquad on\ \partial\Omega_i \times (0,T] \end{cases}$$

$$Flux_i(\lambda, u_i) \cdot n_i = Flux_j(\lambda, u_j) \cdot n_j, \quad on\ \partial\Omega_i \cap \partial\Omega_j \times (0,T]$$

Follows multiscale framework, operators not all directly accessible

$$\frac{\partial u_c}{\partial t} = F_c(u_c, u_f) \qquad \frac{\partial \lambda}{\partial t} = F(\lambda, u_i)$$

$$\frac{\partial u_f}{\partial t} = F_f(u_c, u_f) \qquad \frac{\partial u_i}{\partial t} = F_i(\lambda, u_i)$$

$$\frac{\partial u_c}{\partial t} = F_c(u_c, h(u_c)) \qquad \frac{\partial \lambda}{\partial t} = F(\lambda, h(\lambda))$$

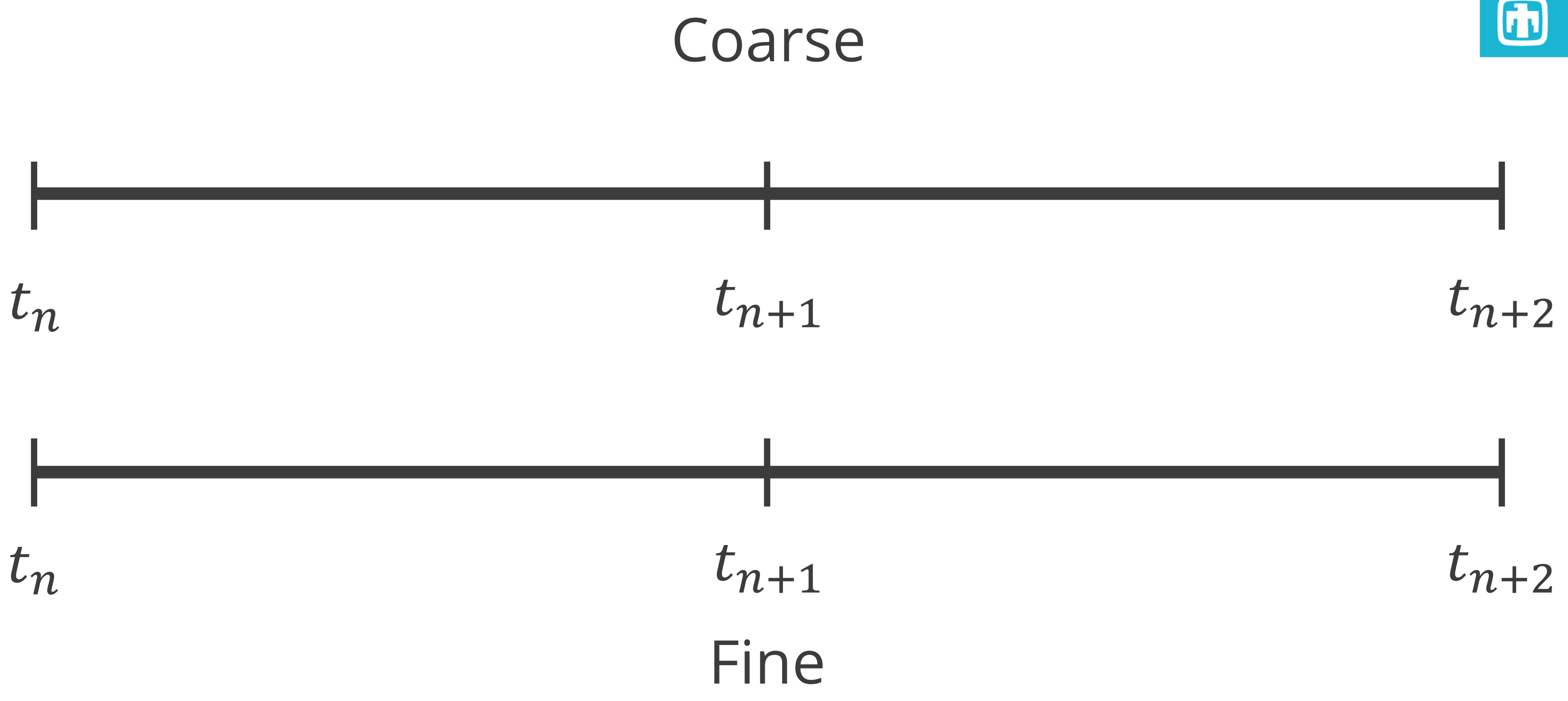
$$\begin{cases} \dfrac{\partial u_i}{\partial t} + \nabla \cdot F(u_i) = G(u_i), & in\ \Omega_i \times (0,T] \\ u_i = \lambda, & on\ \partial\Omega_i \times (0,T] \end{cases}$$

Operator not explicitly known.
Occurs under-the-hood when enforcing flux continuity

$$Flux_i(\lambda, u_i) \cdot n_i = Flux_j(\lambda, u_j) \cdot n_j$$

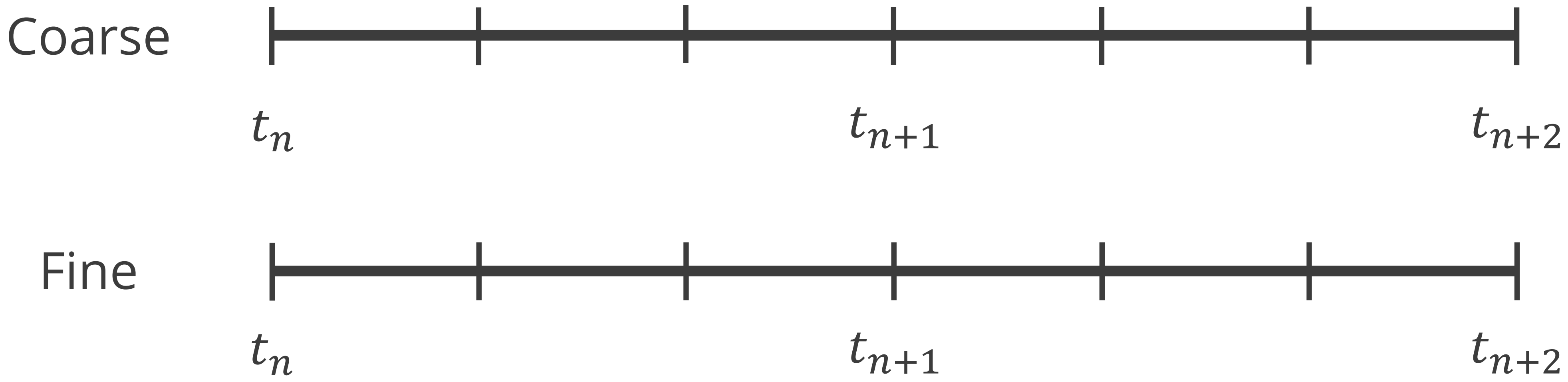
Order matters…

Time discretizing then hybridizing leads to synchronous time stepping



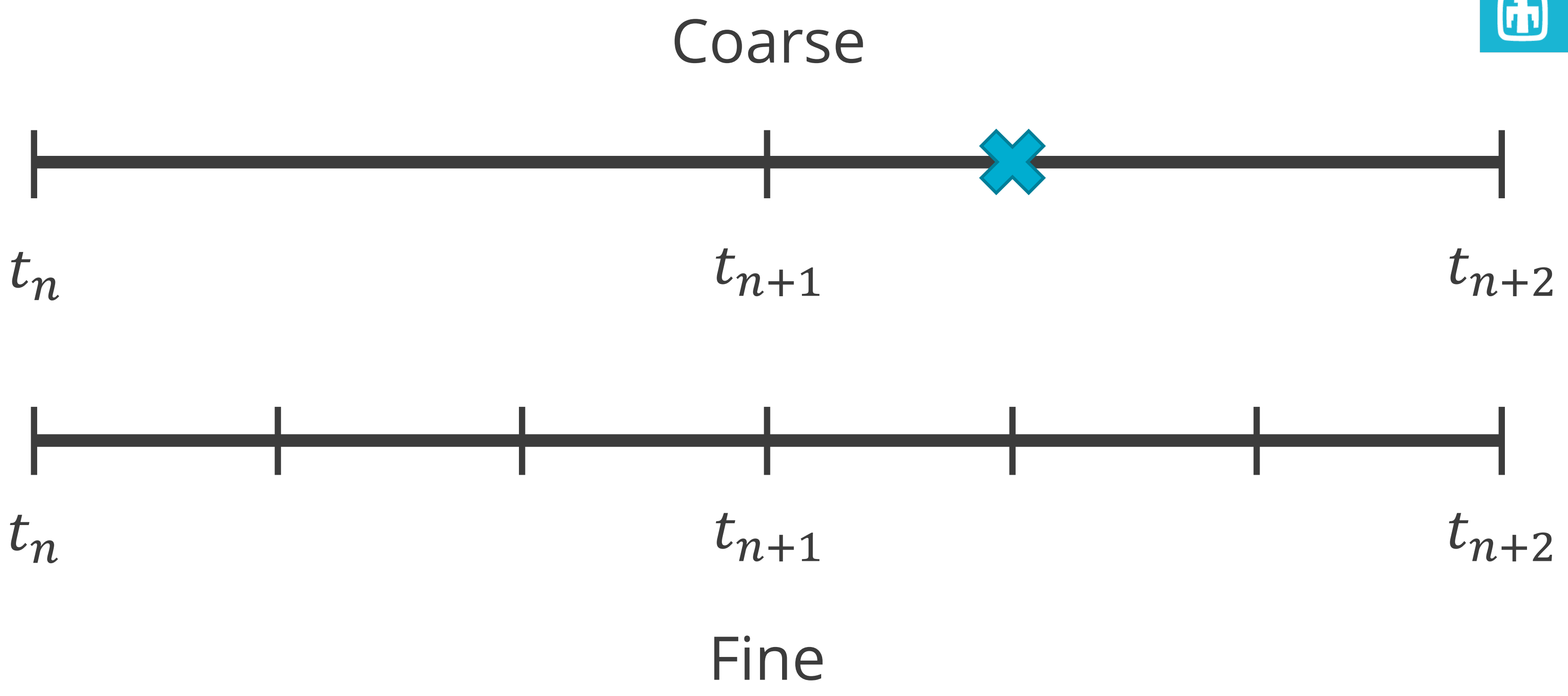
- Time scheme shared by coarsescale and finescale
- Appropriate if timescales are also shared
- Simple to implement
- Clear how to get higher order accuracy
- Global solve required every (sub)stage

Synchronous time advancement



Order matters…

Hybridizing then time discretizing leads to asynchronous time stepping



- Allows for multirate timestepping
- If appropriate, reduces # of global solves
- Overall order limited by coarsescale
- Coarsescale variable needs to be interpolated
- Nuanced implementation

Automatic differentiation for multiscale methods

- MrHyDE only evaluates residuals, obtains Jacobians through automatic differentiation and forward sensitivity
- Easy to add and couple new physics modules
- Explicit form of "macro-micro-macro" map not necessary
- Much more accurate and efficient than finite difference
- Sensitivity needs to be propagated through microscale model
- More difficult in asynchronous transient case

MrHyDE

Numerical Results

Asynchronous Backward Euler with finescale substepping more accurate

Consider a simple model for heat transport

$$\frac{\partial u}{\partial t} - \nabla \cdot (\mathbb{K}\nabla u) = f(x,t),$$

and choose source term, boundary and initial conditions so that,

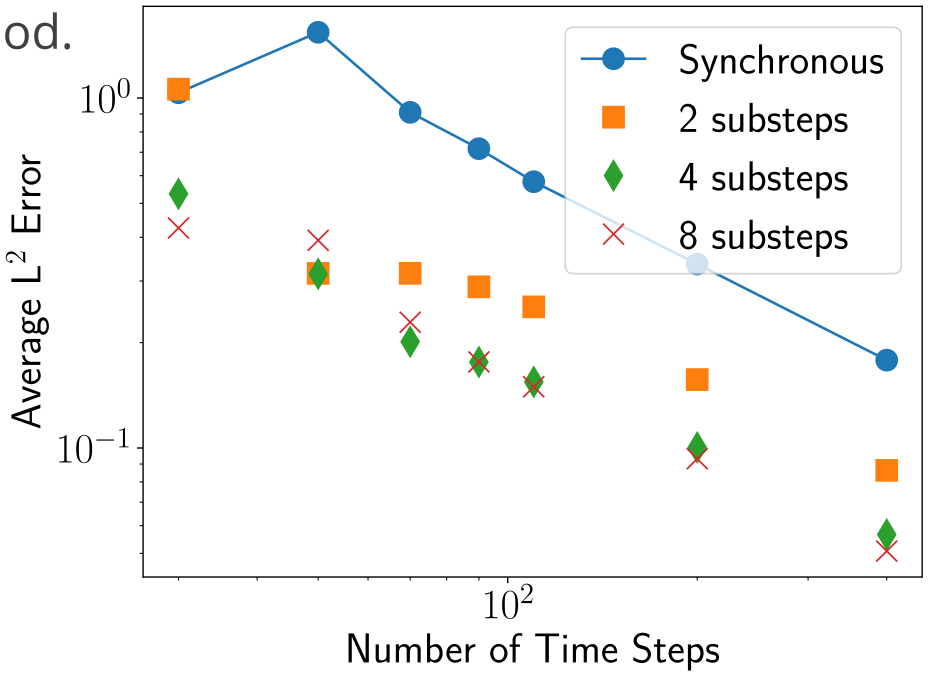
$$u(x,t) = (\sin(\pi t) + \cos(20\pi t))\sin(\pi x)\sin(\pi y).$$

Notes:

Used a hybridized IPDG method.

Spatial disc.: PW linear, 32^2

BWE time stepping



Asynchronous Scheme Enables Novel Implicit/Explicit (IMEX) Methods

Consider a simple model for heat transport

$$\frac{\partial u}{\partial t} - \nabla \cdot (\mathbb{K}\nabla u) = f(x,t),$$

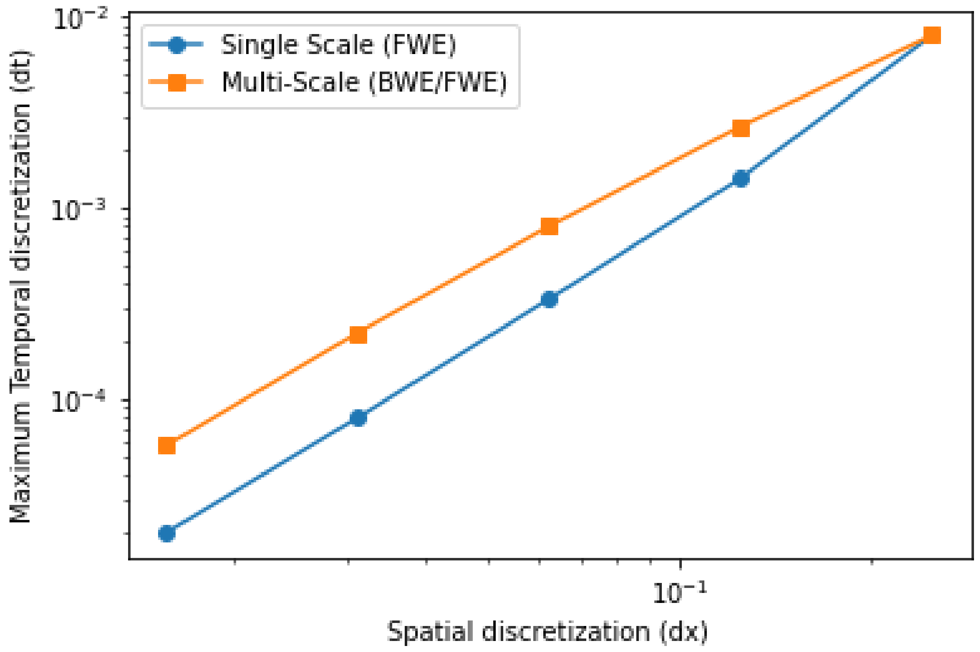
$f = 1$, $u(x,0)$, homogeneous Dirichlet boundary conditions.

Compare maximum stable time step size for two schemes:

Single-scale FWE

Multi-scale BWE/FWE

- Implicit global problem
- Explicit local problem



Multirate Time Stepping Can Be Combined with Other Capabilities – Dynamic Adaptive Subgrid Modeling

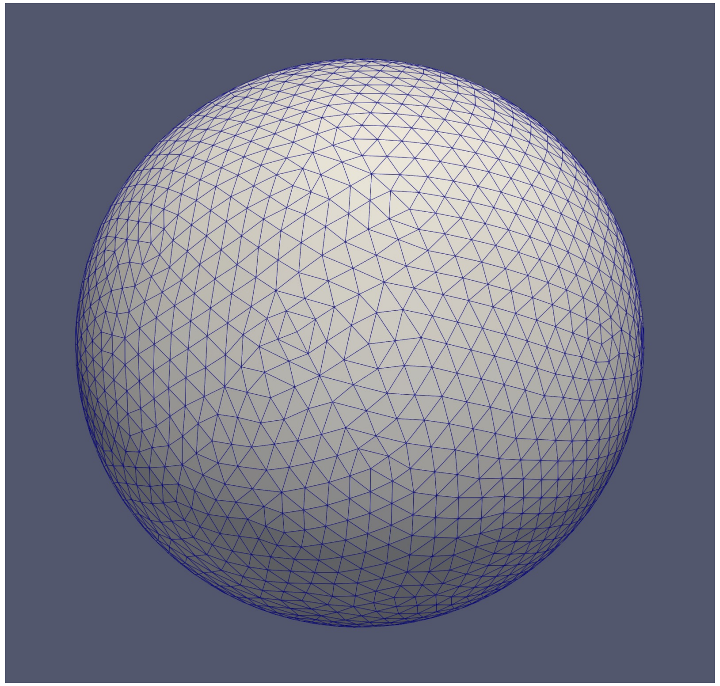
Multiscale HDG framework allows tremendous flexibility

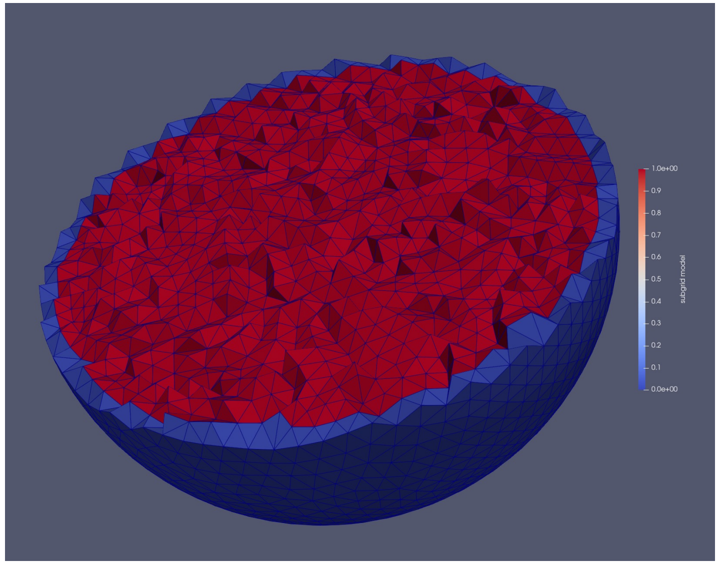
Local high-resolution time stepping can be applied in specific regions

- Boundary layer to resolve a high-frequency boundary condition

How to choose which subgrid model to use in each coarse scale element?

- Region-adaptive (see figure)
- Solution-adaptive
- Error estimation (hierarchical or *a posteriori*)
- Machine Learning (see T. Wildey's presentation – MS805)





Conclusions

Conclusions and future work

- Room to make significant progress for timestepping in HFE framework
- Natural to pursue more flexible schemes for multiscale/multiphysics problems

- Develop a framework to perform analysis of HFE systems
  - Challenge is understanding structure of macro-micro-macro map
- Can more general time integration strategies increase efficiency/stability?
- Always looking to push HFE methods to become more practical/tractable