

A Quasi-Static Projection Method for 3-Dimensional Hypoelastoplasticity

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Harvard University, Department of Applied Mathematics.

Rycroft Group.

Bulk Metallic Glasses

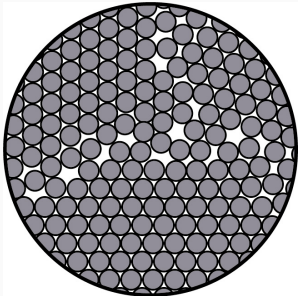
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- **Amorphous** structure gives unique properties.

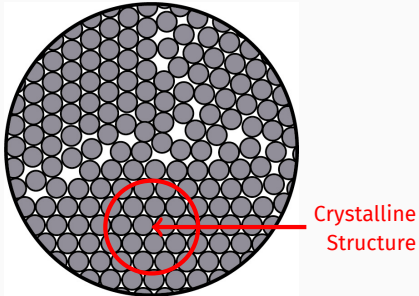
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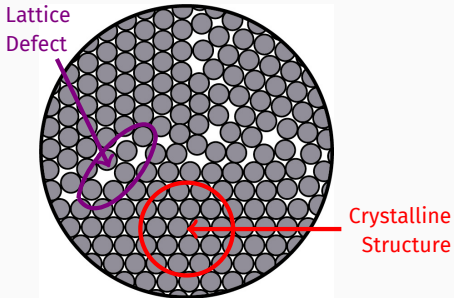
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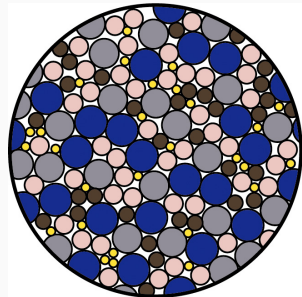
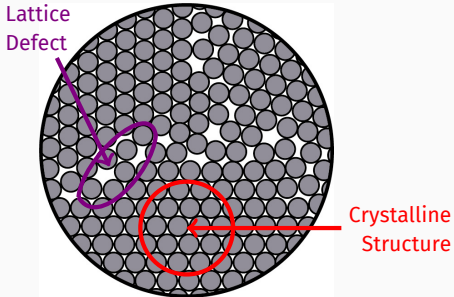
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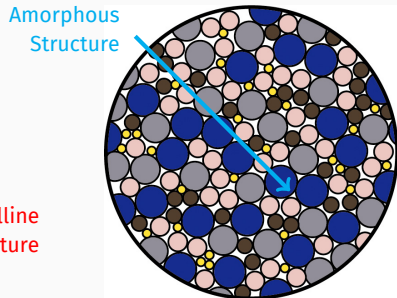
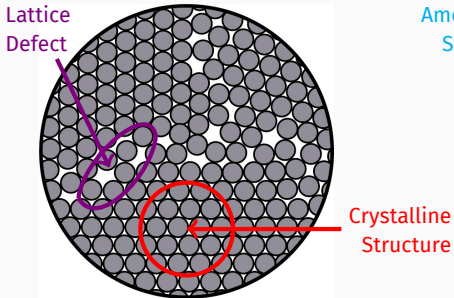
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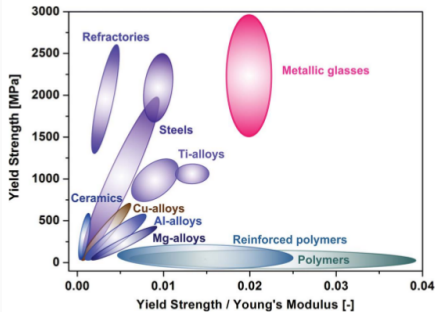
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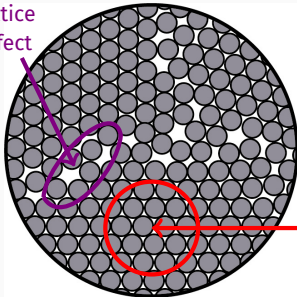


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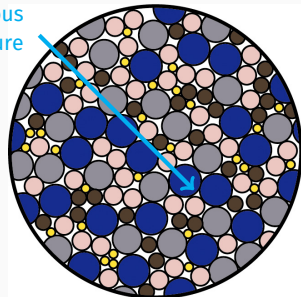


Lattice Defect



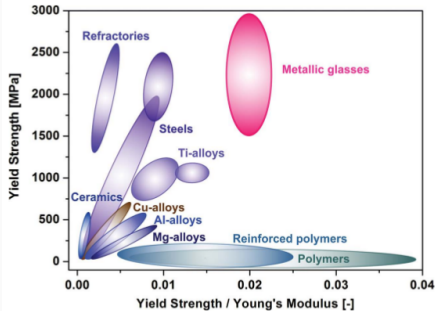
Crystalline Structure

Amorphous Structure

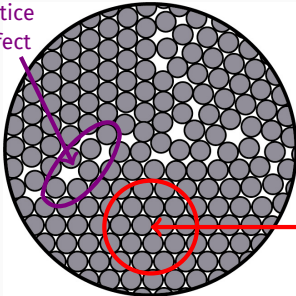


Bulk Metallic Glasses

- Solid metal with atoms “frozen” into liquid-like **disorder**.
- **Amorphous** structure gives unique properties.
- Catastrophic failure: **shear banding**.

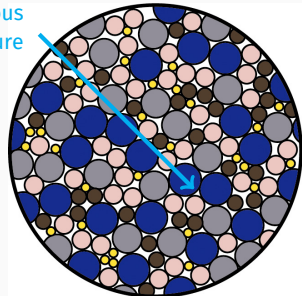


Lattice Defect



Crystalline Structure

Amorphous Structure



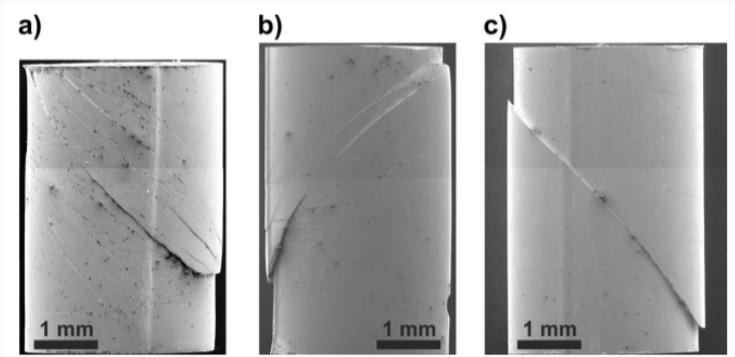
- Localization of stress due to localization of strain.

Shear Bands

- Localization of stress due to localization of strain.
- Strain-softening instability provides positive feedback.

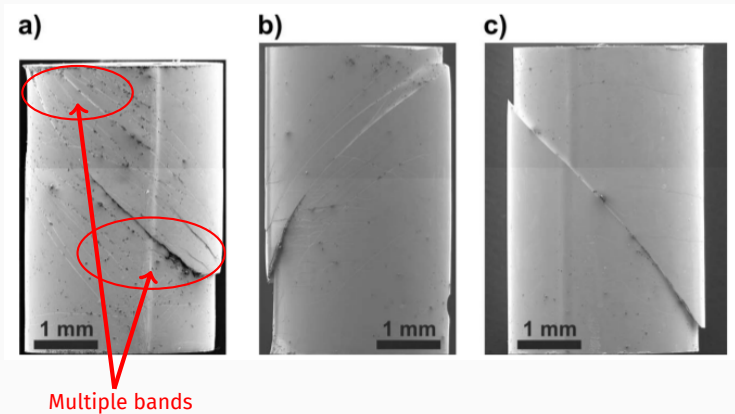
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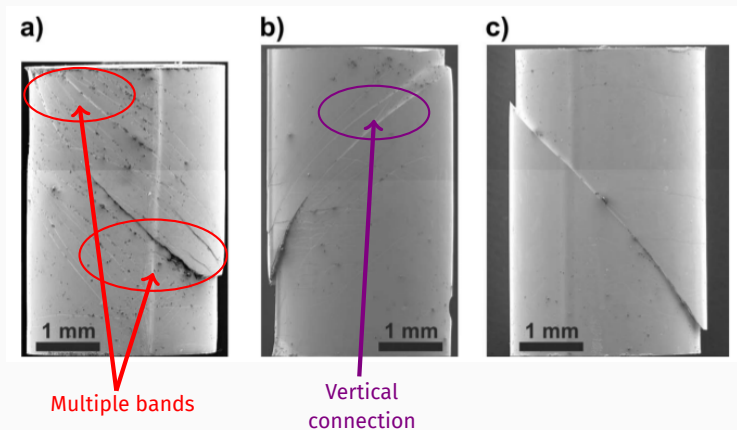
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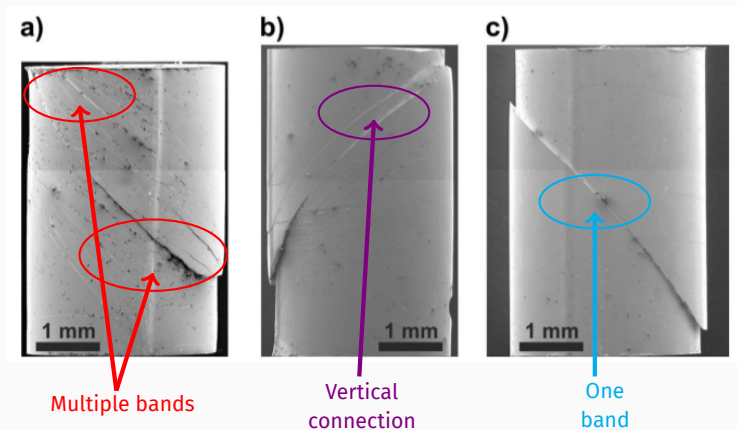
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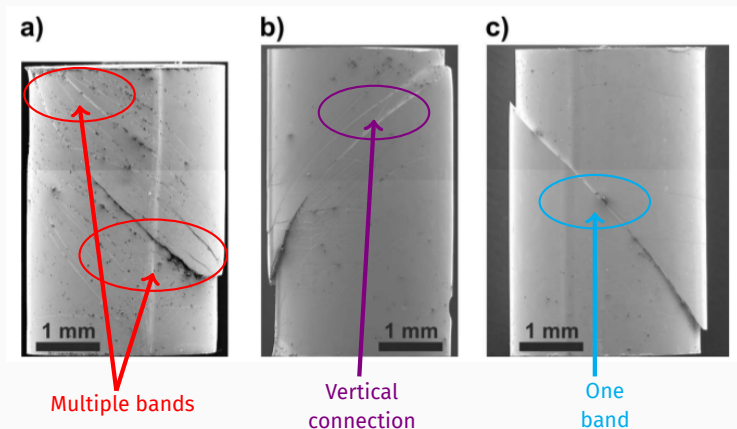
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Shear Bands

- Localization of stress due to localization of strain.
- Strain-softening instability provides positive feedback.
- Effective temperature χ quantifies localized “softness”.



Linear Elasticity

Shear Transformation Zone Theory

Linear Elasticity

$$\frac{\mathcal{D}\sigma}{\mathcal{D}t} = \mathbf{C} : \mathbf{D}^{\text{el}}$$

Shear Transformation Zone Theory

Linear Elasticity

$$\underbrace{\frac{\mathcal{D}\sigma}{\mathcal{D}t}} = \mathbf{C} : \mathbf{D}^{\text{el}}$$

Jaumann derivative

Shear Transformation Zone Theory

Linear Elasticity

$$\underbrace{\frac{\mathcal{D}\sigma}{\mathcal{D}t}}_{\text{Jaumann derivative}} = \overset{\text{Stiffness}}{\hat{\mathbf{C}}} : \mathbf{D}^{\text{el}}$$

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$$= \mathbf{D}^{el} + \mathbf{D}^{pl}$$

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Hypoelastoplastic **assumption**

Shear Transformation Zone Theory

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Hypoelastoplastic **assumption**

$$\rho \frac{d\mathbf{u}}{dt} = \nabla \cdot \boldsymbol{\sigma}$$

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Hypoelastoplastic **assumption**

$$\underbrace{\rho \frac{d\mathbf{u}}{dt}}_{m \times a} = \underbrace{\nabla \cdot \boldsymbol{\sigma}}_{\text{Net force}}$$

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Shear Transformation Zone Theory

$$\frac{d\chi}{dt} = \frac{D^{pl} \bar{s}}{s_y c_0} (\chi_\infty - \chi)$$

Linear Elasticity

$$\underbrace{\frac{D\sigma}{Dt}}_{\text{Jaumann derivative}} = \underbrace{\bar{\mathbf{C}}}_{\text{Stiffness}} : \underbrace{\mathbf{D}}_{\text{Elastic Part}}^{el}$$

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$$\bar{s}^2 = \frac{1}{2} \sigma_{0,ij} \sigma_{0,ij}$$

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$$\text{Total deviatoric stress } \underbrace{\bar{s}^2}_{\text{Total deviatoric stress}} = \frac{1}{2} \sigma_{0,ij} \sigma_{0,ij}$$

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Linear Elasticity

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$$\begin{aligned} \text{Rate of deformation } \mathbf{D} &= \underbrace{\frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)}_{\text{Definition}} \\ &= \underbrace{\mathbf{D}^{el} + \mathbf{D}^{pl}}_{\text{Hypoelastoplastic assumption}} \end{aligned}$$

$$\underbrace{\rho \frac{d\mathbf{u}}{dt}}_{m \times a} = \underbrace{\nabla \cdot \boldsymbol{\sigma}}_{\text{Net force}}$$

Shear Transformation Zone Theory

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$$\sigma_0 = \sigma - \frac{1}{3} \text{Tr}(\sigma) \mathbf{I}$$

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$$\text{Plastic rate } \mathbf{D}^{pl} = D^{pl} \frac{\sigma_0}{s}$$

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A Thought-Provoking Analogy

Hypoelastoplastic Long-Time Limit

Incompressible Navier-Stokes

From Navier-Stokes to Hypoelastoplasticity

A Thought-Provoking Analogy

Hypoelastoplastic Long-Time Limit

$$\frac{\mathcal{D}\sigma}{\mathcal{D}t} = \mathbf{C} : (\mathbf{D} - \mathbf{D}^{pl})$$

Incompressible Navier-Stokes

From Navier-Stokes to Hypoelastoplasticity

A Thought-Provoking Analogy

Hypoelastoplastic Long-Time Limit

$$\underbrace{\frac{\mathcal{D}\sigma}{\mathcal{D}t} = \mathbf{C} : (\mathbf{D} - \mathbf{D}^{pl})}_{\text{Hypoelastoplastic equation}}$$

Incompressible Navier-Stokes

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Incompressible Navier-Stokes

$$\rho \frac{d\mathbf{u}}{dt} = -\nabla p + \nabla \cdot \mathbf{T}$$

From Navier-Stokes to Hypoelastoplasticity

A Thought-Provoking Analogy

Hypoelastoplastic Long-Time Limit

$$\frac{\mathcal{D}\sigma}{\mathcal{D}t} = \mathbf{C} : (\mathbf{D} - \mathbf{D}^{pl})$$

Hypoelastoplastic equation

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Navier-Stokes equation

From Navier-Stokes to Hypoelastoplasticity

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Hypoelastoplastic Long-Time Limit

$$\underbrace{\frac{\mathcal{D}\sigma}{\mathcal{D}t} = \mathbf{C} : (\mathbf{D} - \mathbf{D}^{pl})}_{\text{Hypoelastoplastic equation}}$$

$$\nabla \cdot \sigma \approx 0$$

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$$\underbrace{\nabla \cdot \mathbf{u} \approx 0}_{\text{Incompressibility constraint}}$$

From Navier-Stokes to Hypoelastoplasticity

A Thought-Provoking Analogy

Hypoelastoplastic Long-Time Limit

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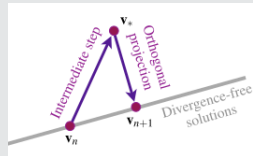
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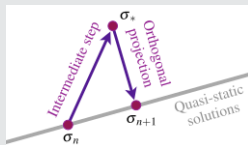
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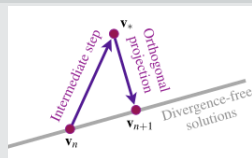
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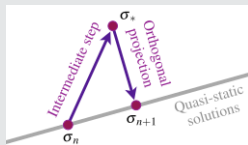
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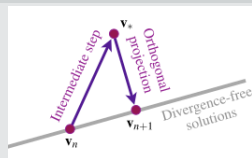
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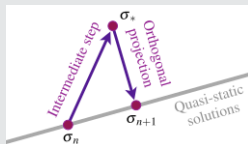
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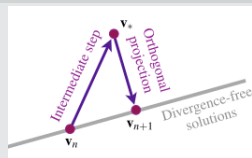
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Forward-Euler intermediate step

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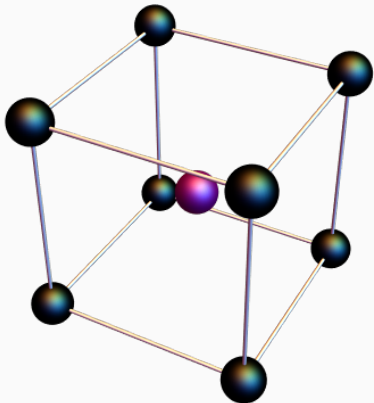
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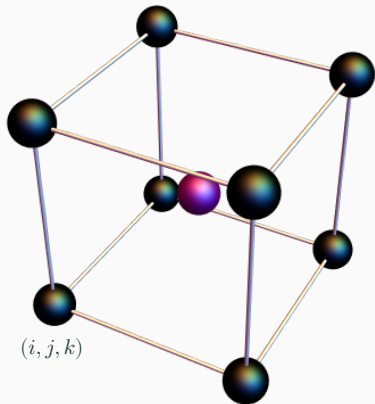
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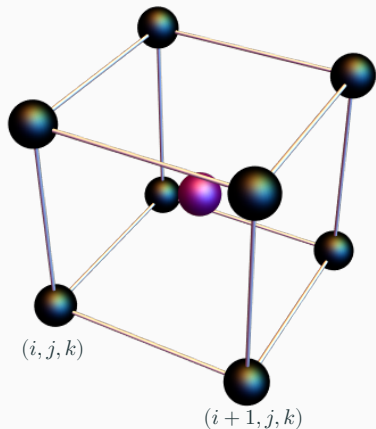
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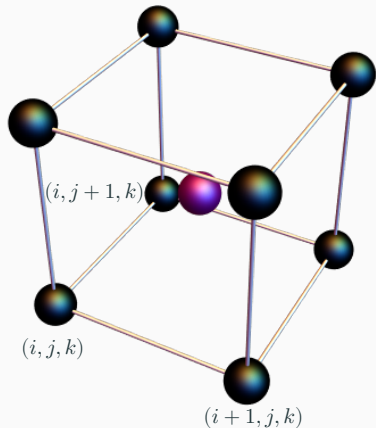
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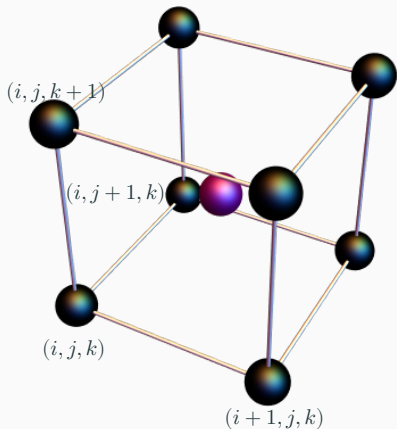
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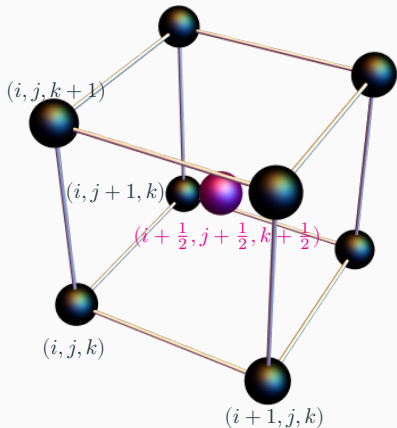
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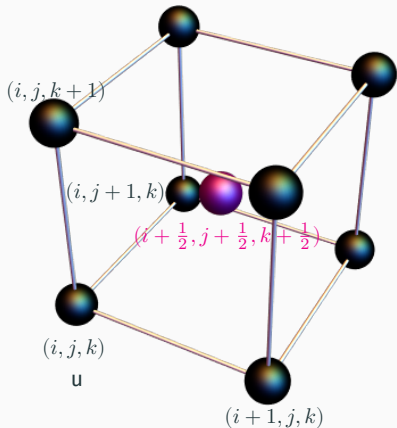
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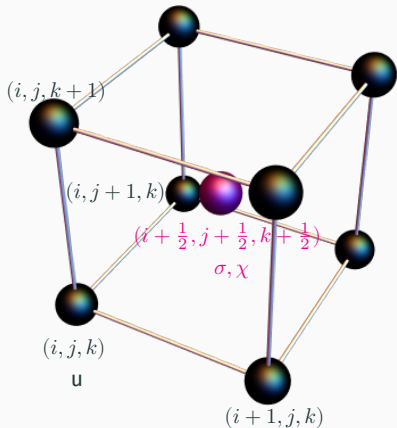
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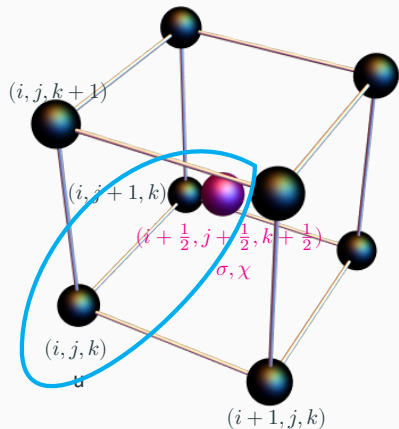
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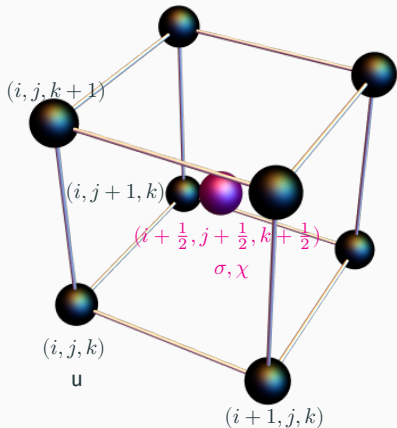
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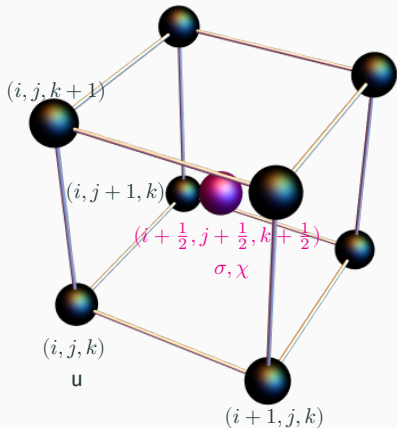
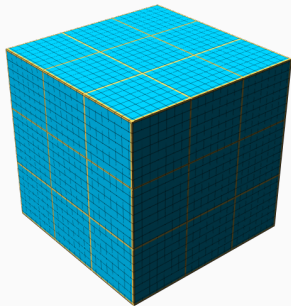
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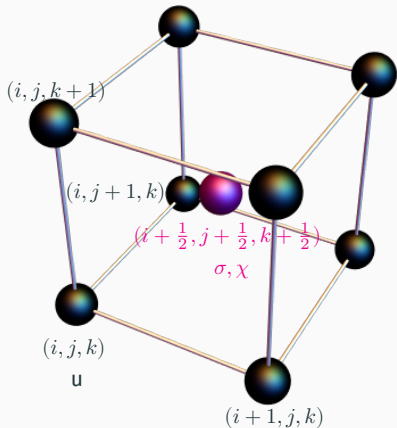
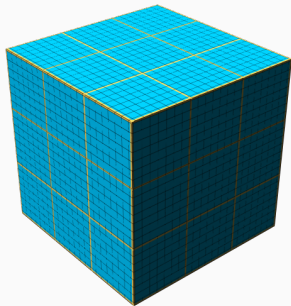
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Projection Step

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superscript: iteration count

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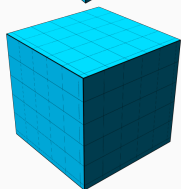
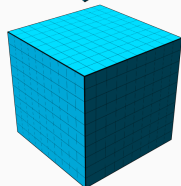
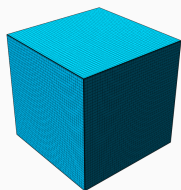
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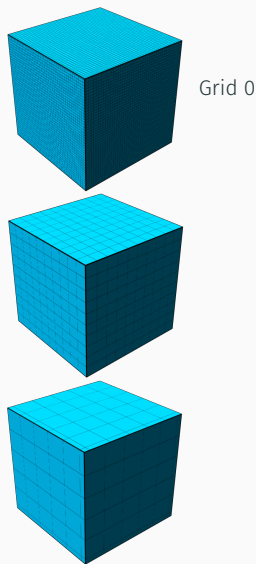
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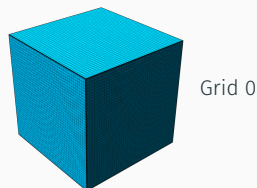
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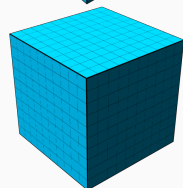
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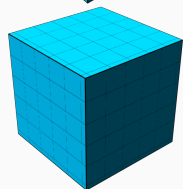
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Grid 0



Grid 1



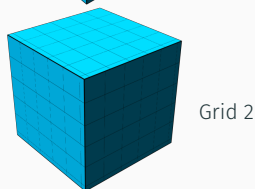
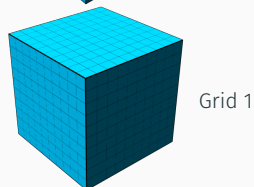
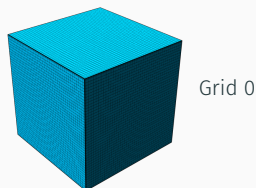
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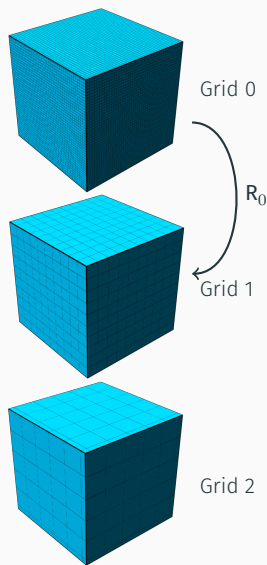
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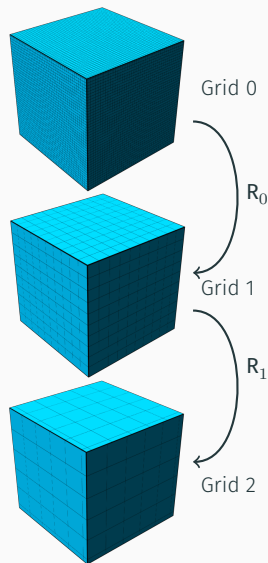
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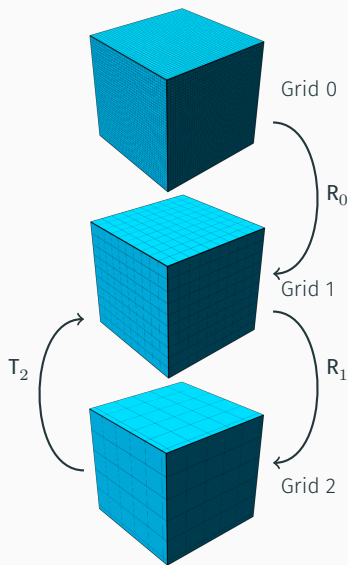
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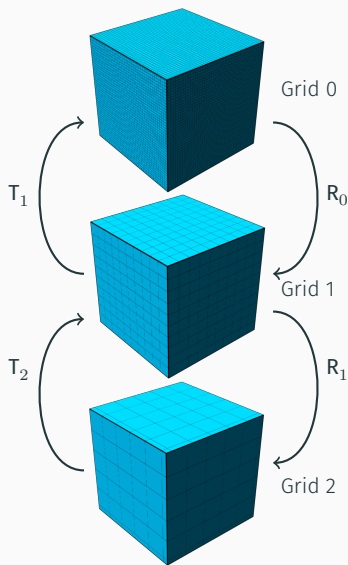
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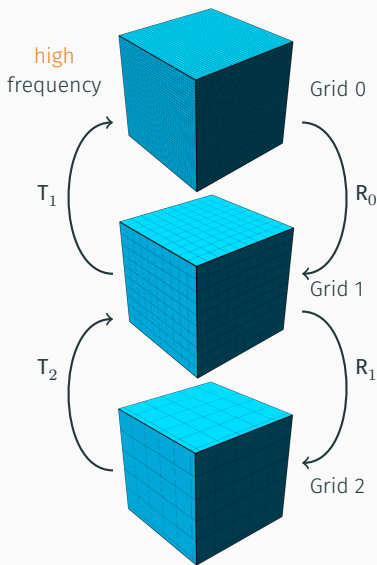
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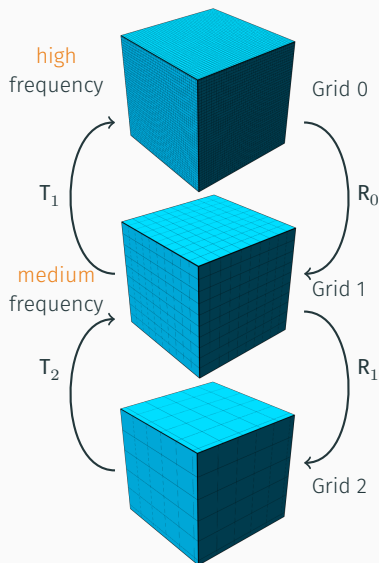
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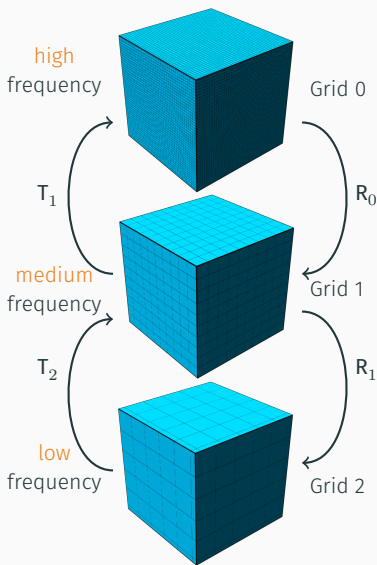
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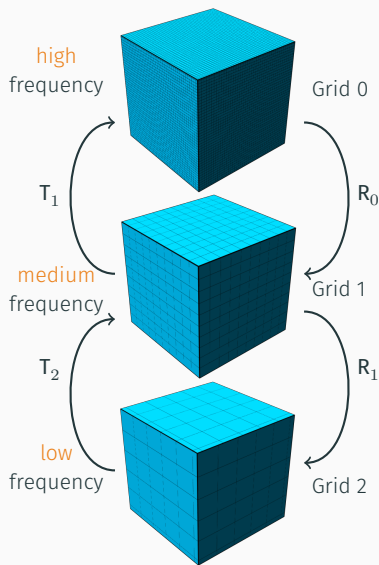
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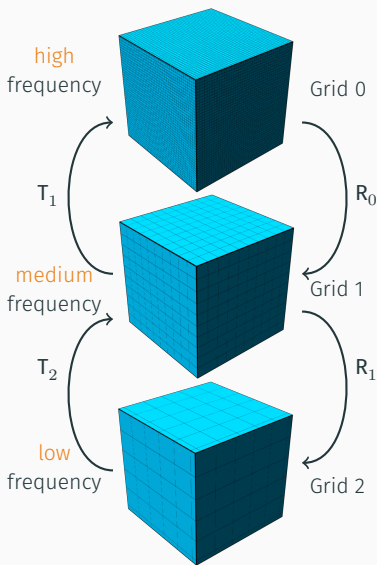
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- C++ templates to solve for arbitrary datatypes (n -dimensional vectors, complex numbers, etc.) at each point.



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1D Example

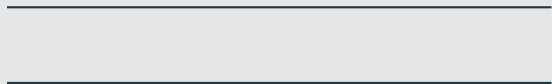
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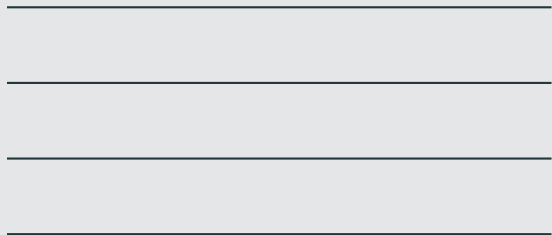
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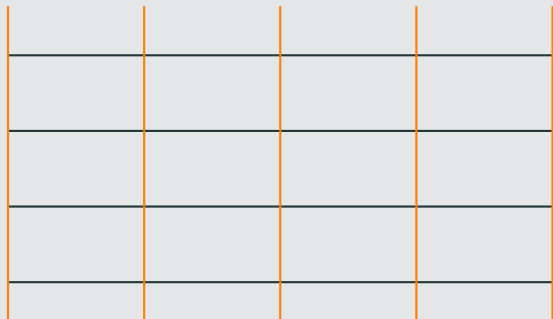
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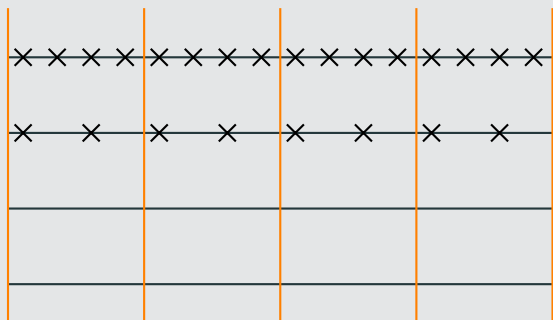


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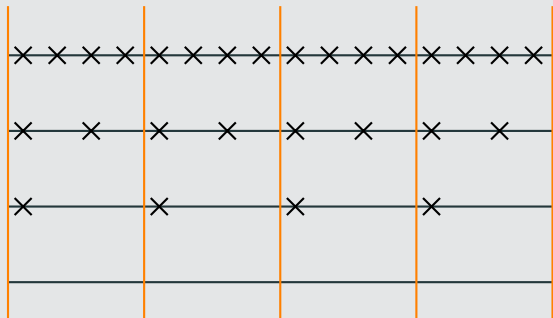
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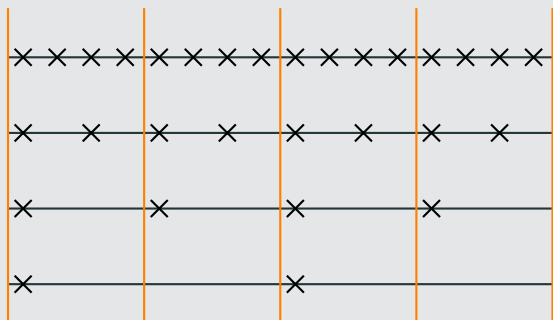
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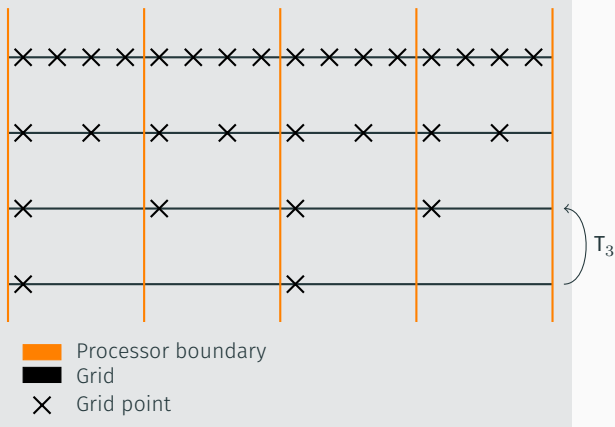
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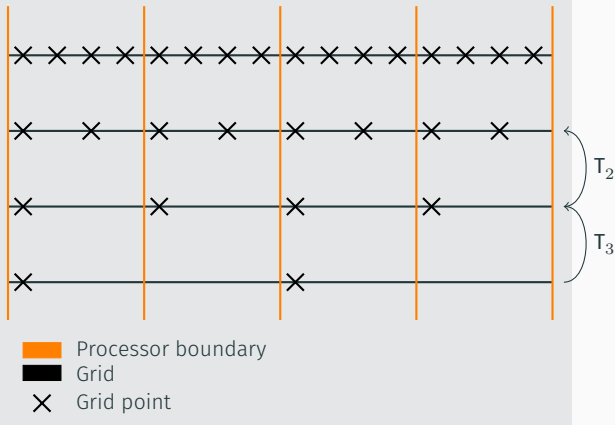
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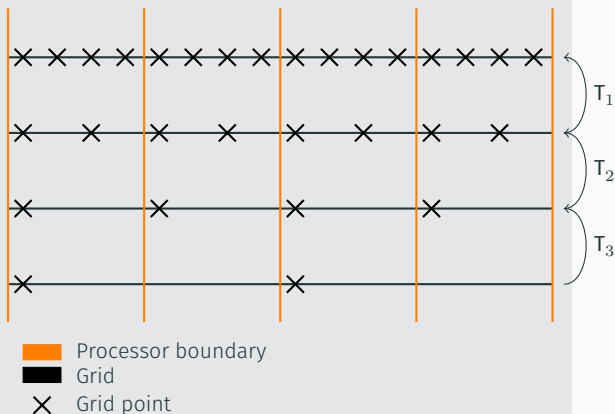
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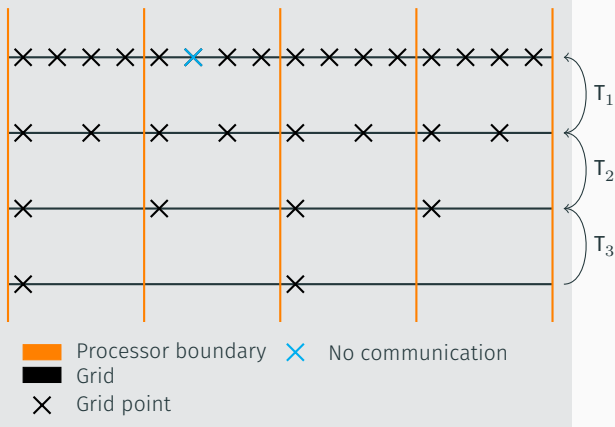
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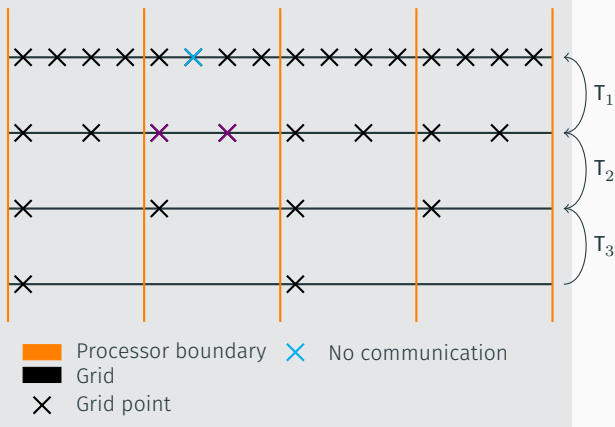
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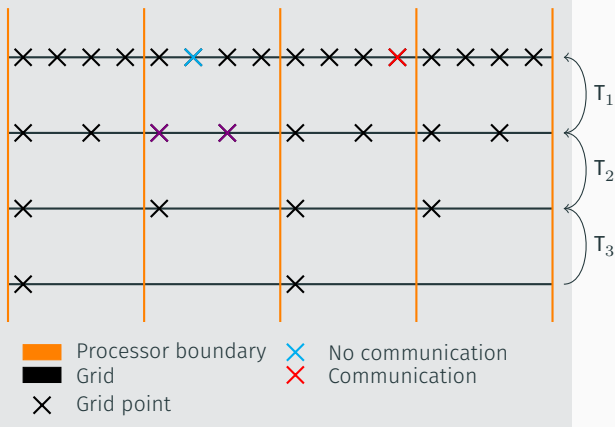
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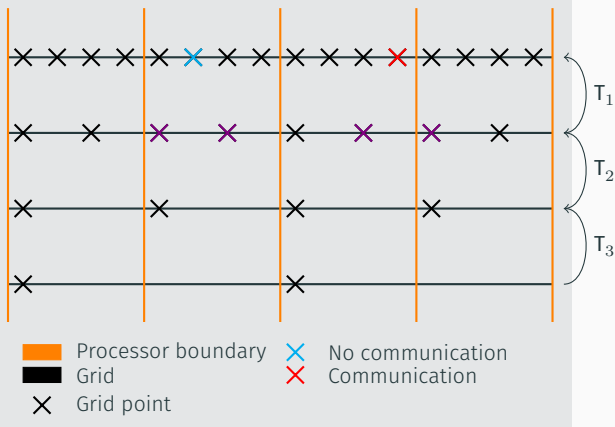
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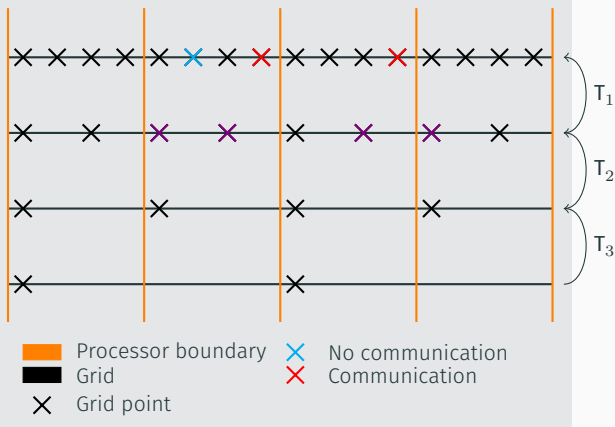
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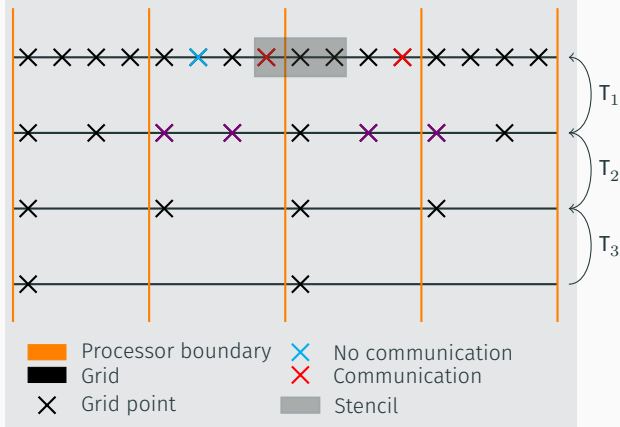
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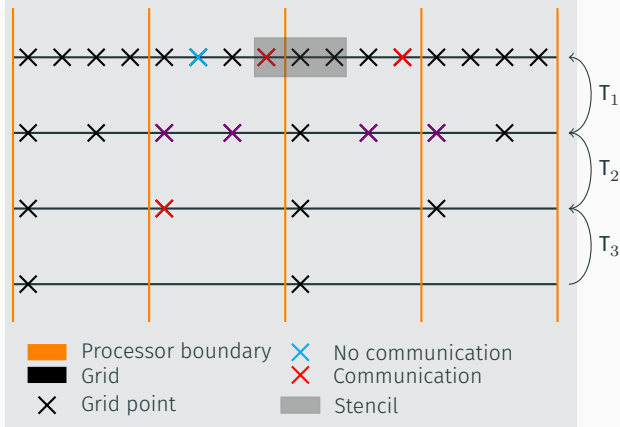
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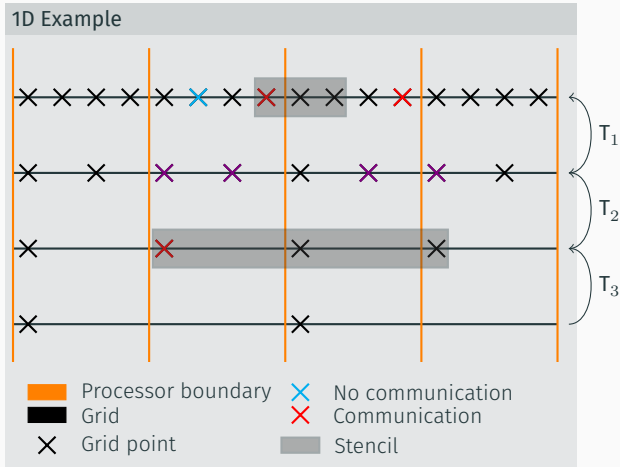
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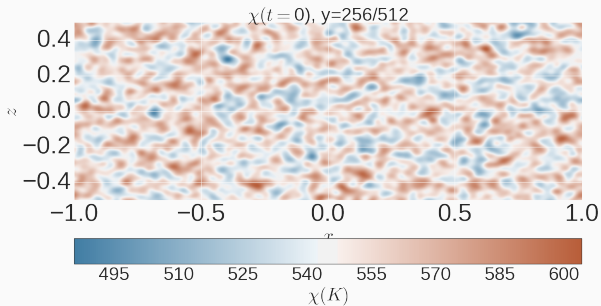
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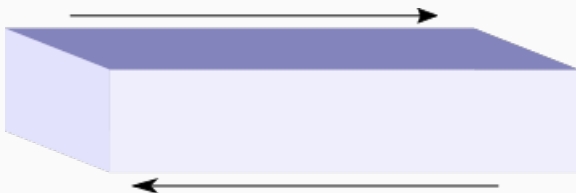
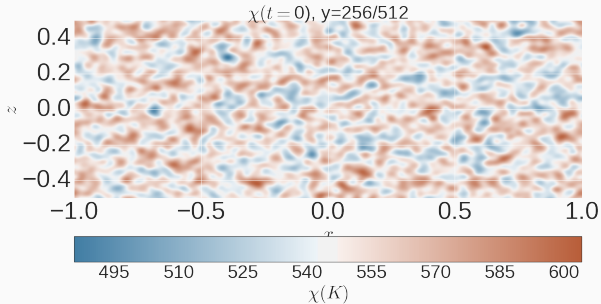
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Quasi-Static Results

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- Thanks to Chris Rycroft, collaborators Eran Bouchbinder, Michael Falk, Michael Shields, and the Department of Energy Computational Science Graduate Fellowship for funding.