

**MAP 2320 – MÉTODOS NUMÉRICOS EM EQUAÇÕES
DIFERENCIAIS II**

2º Semestre - 2020

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A Guide to Numerical Methods for Transport Equations

2010

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Mathematics of Transport Phenomena

$$\frac{\partial}{\partial t} \int_V u(\mathbf{x}, t) d\mathbf{x} + \int_S \mathbf{f} \cdot \mathbf{n} ds = \int_V s(\mathbf{x}, t) d\mathbf{x}.$$

Quantidade conservada

Fluxo da quantidade conservada

Fonte (ou sumidouro) da
quantidade conservada

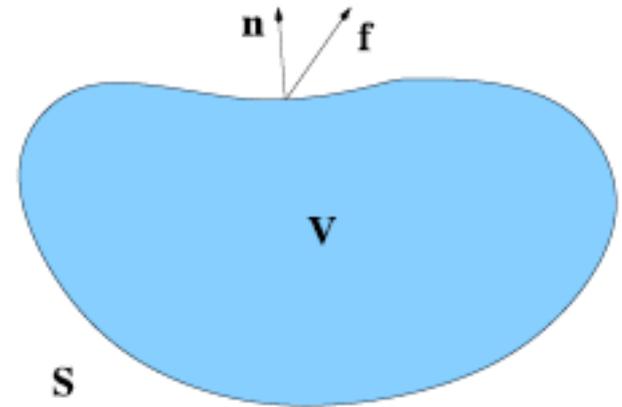


Fig. 1.1 A fixed control volume V bounded by the control surface S .

Massa – Quantidade de Movimento - Energia

If the functions $u(\mathbf{x}, t)$ and $\mathbf{f}(\mathbf{x}, t)$ are differentiable, then the divergence theorem, as applied to the surface integral in (1.2), yields the identity

$$\int_V \left[\frac{\partial u(\mathbf{x}, t)}{\partial t} + \nabla \cdot \mathbf{f}(\mathbf{x}, t) - s(\mathbf{x}, t) \right] d\mathbf{x} = 0.$$

Since the choice of V is arbitrary, the expression in the square brackets must vanish, so the evolution of $u(\mathbf{x}, t)$ is governed by the partial differential equation (PDE)

$$\frac{\partial u(\mathbf{x}, t)}{\partial t} + \nabla \cdot \mathbf{f}(\mathbf{x}, t) = s(\mathbf{x}, t). \quad (1.3)$$

massa transportada

Gradiente de concentração

In general, both convective and diffusive effects must be taken into account, so

$$\mathbf{f}(\mathbf{x}, t) = \mathbf{v}(\mathbf{x}, t)u - \mathcal{D}(\mathbf{x}, t)\rho \nabla c. \quad (1.7)$$

However, the rates of convective and diffusive transport may be quite different. For example, the transport of pollutants in a river is dominated by convection, whereas the spreading of pollutants in a lake is dominated by diffusion (dispersion).

Velocidade de transporte

Coeficiente de difusão

Convecção
Ou
Advecção

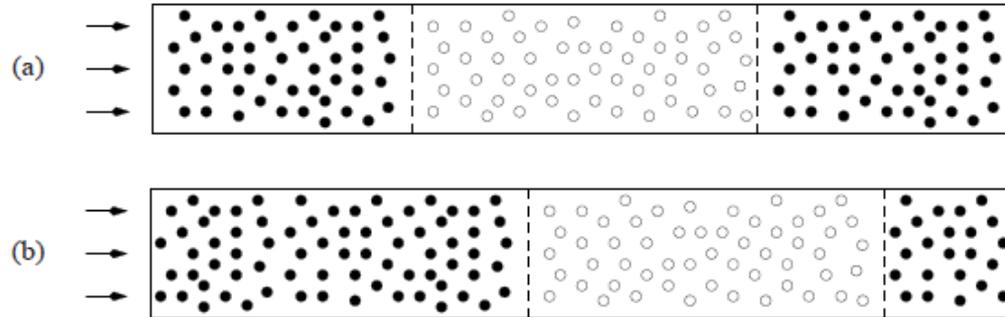


Fig. 1.2 Transport of tracer particles in a pipe filled with moving water.

Difusão

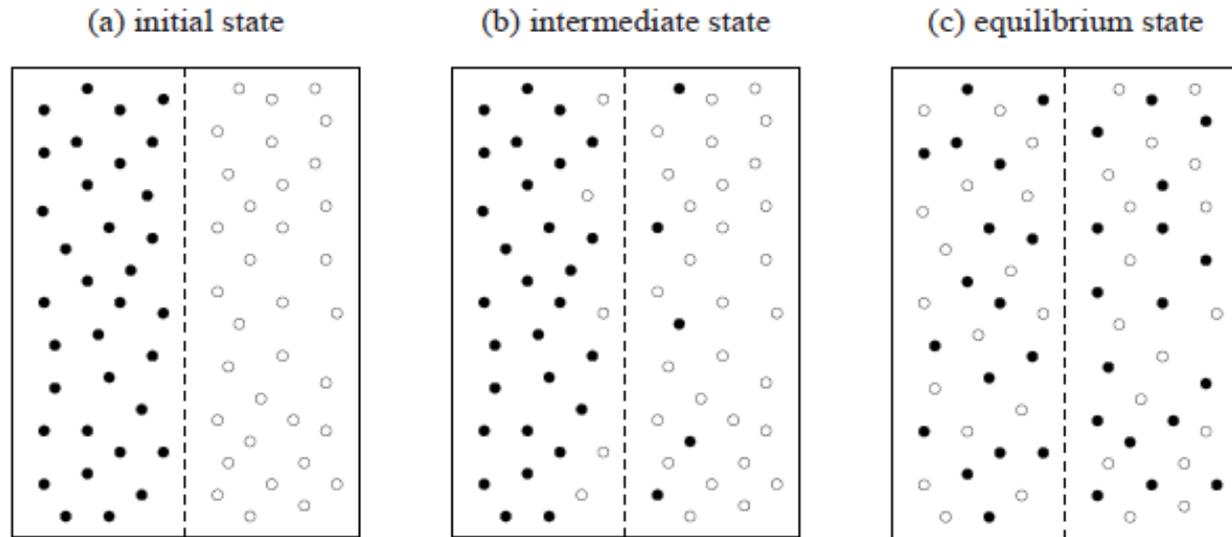


Fig. 1.3 Random motion of molecules across an interface in a stationary liquid.

The Generic Transport Equation

$$\frac{\partial \rho c}{\partial t} + \nabla \cdot (\mathbf{v} \rho c) - \nabla \cdot (\mathcal{D} \rho \nabla c) = s.$$

- the rate-of-change term $\frac{\partial \rho c}{\partial t}$ is the net gain/loss of mass per unit volume and time;
- the convective term $\nabla \cdot (\mathbf{v} \rho c)$ is due to the downstream transport with velocity \mathbf{v} ;
- the diffusive term $-\nabla \cdot (\mathcal{D} \rho \nabla c)$ is due to a nonuniform spatial distribution of c ;
- the source or sink term s combines all other effects that create or destroy ρc .

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v} u) - \nabla \cdot (\mathcal{D} \nabla u) = s.$$

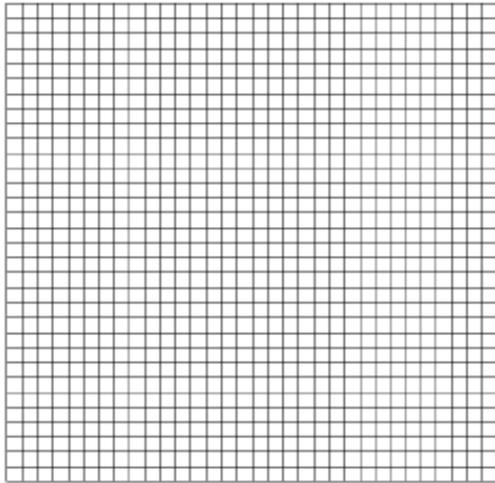
convection-diffusion-reaction (CDR) equation

Summary of Model Problems

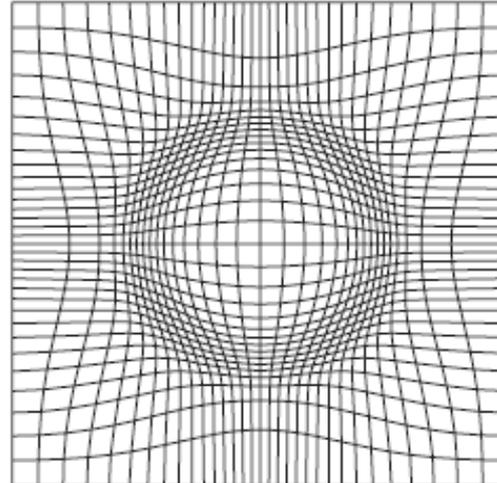
Table 1.1 Summary of models for convection, diffusion, and reaction processes.

PDE type	multidimensional	one-dimensional
elliptic	$\nabla \cdot (\mathbf{v}u - \mathcal{D}\nabla u) = s$ $-\nabla \cdot (\mathcal{D}\nabla u) = s$	$v\frac{\partial u}{\partial x} - d\frac{\partial^2 u}{\partial x^2} = s$ $-d\frac{\partial^2 u}{\partial x^2} = s$
hyperbolic	$\nabla \cdot (\mathbf{v}u) = s$ $\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) = s$	$v\frac{\partial u}{\partial x} = s$ $\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = s$
parabolic	$\frac{\partial u}{\partial t} - \nabla \cdot (\mathcal{D}\nabla u) = s$ $\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u - \mathcal{D}\nabla u) = s$	$\frac{\partial u}{\partial t} - d\frac{\partial^2 u}{\partial x^2} = s$ $\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} - d\frac{\partial^2 u}{\partial x^2} = s$

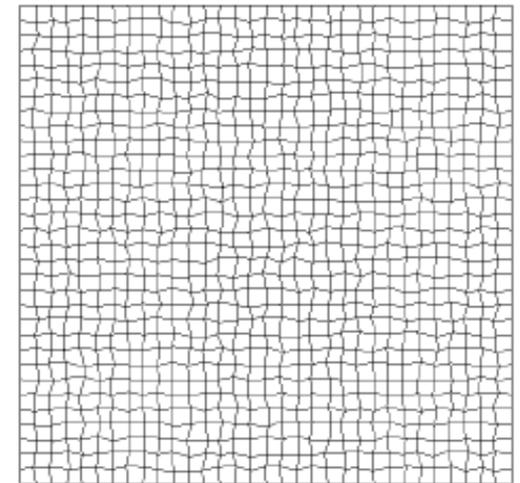
(a) structured, uniform



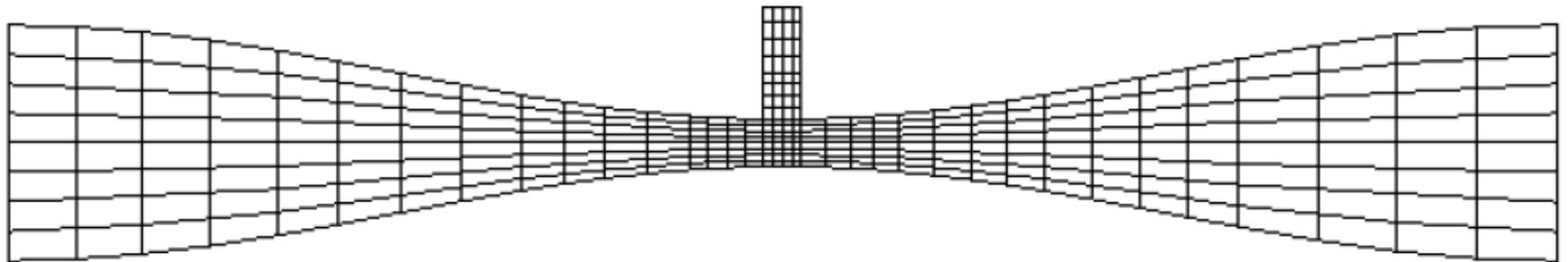
(b) structured, deformed



(c) structured, perturbed

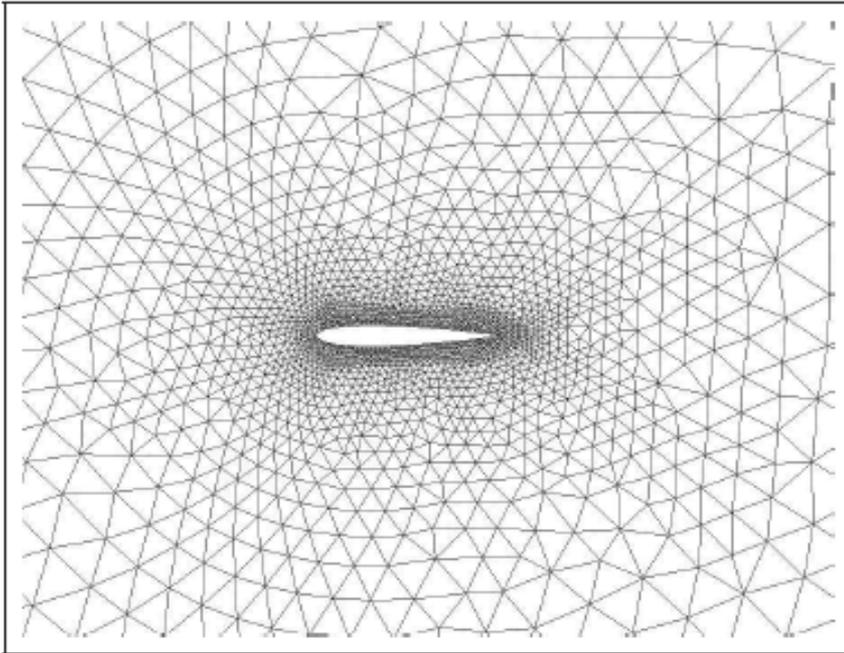


(d) block-structured, 2 subdomains

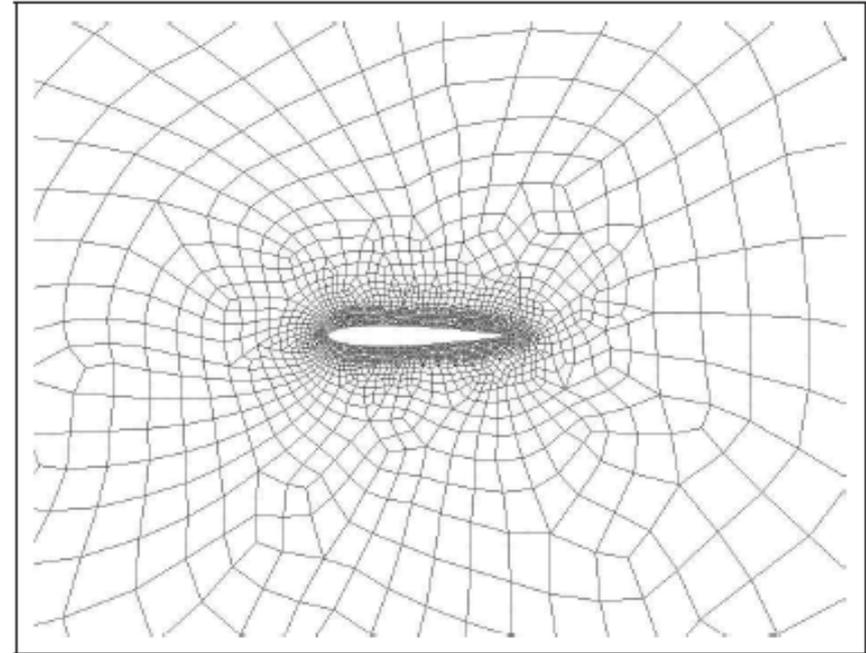


Domínios que podem ser mais facilmente mapeados no quadrado são mais propensos a aplicação do métodos de diferenças finitas.

(e) unstructured, triangular



(f) unstructured, quadrilateral



Domínios mais complexos não podem facilmente ser discretizados de forma a aplicar o método de diferenças finitas. Formulações mais gerais como o método dos Volumes Finitos e o método dos Elementos Finitos são capazes de lidar com discretizações em polígonos.

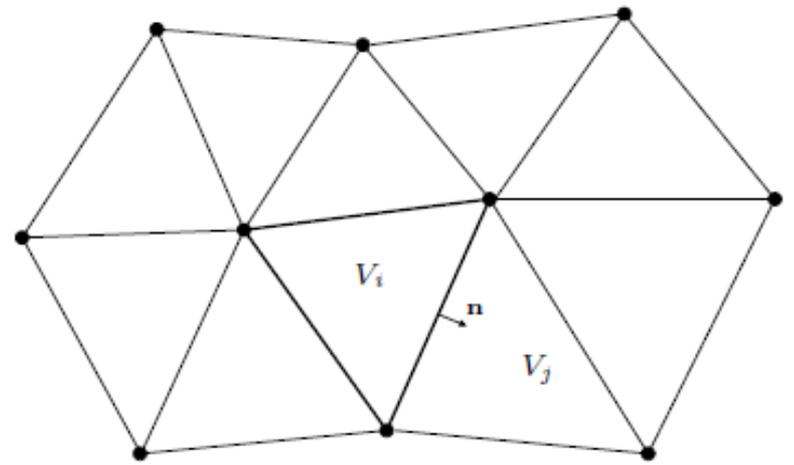
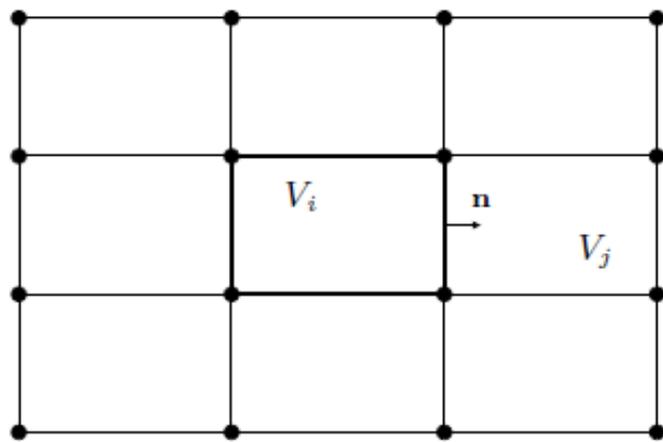


Fig. 1.5 Control volumes for a cell-centered FVM in two dimensions.

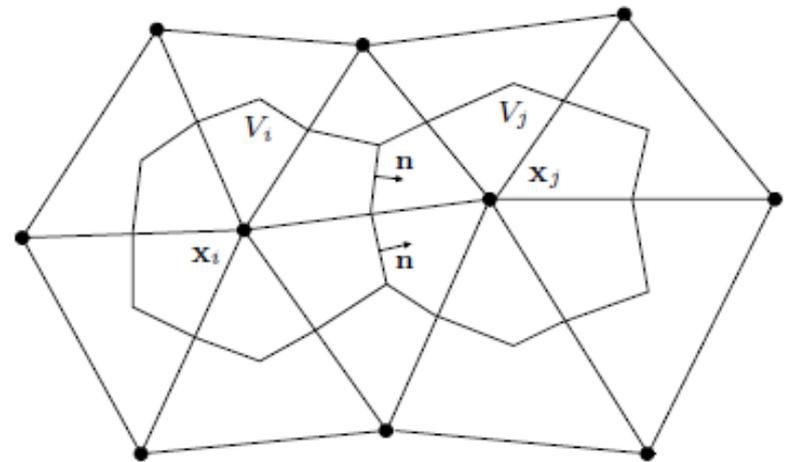
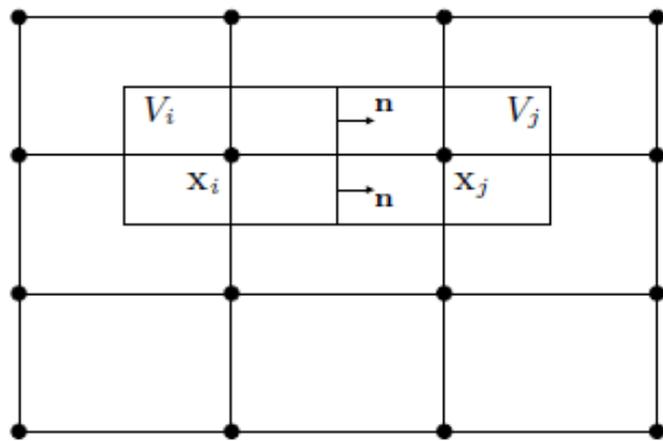
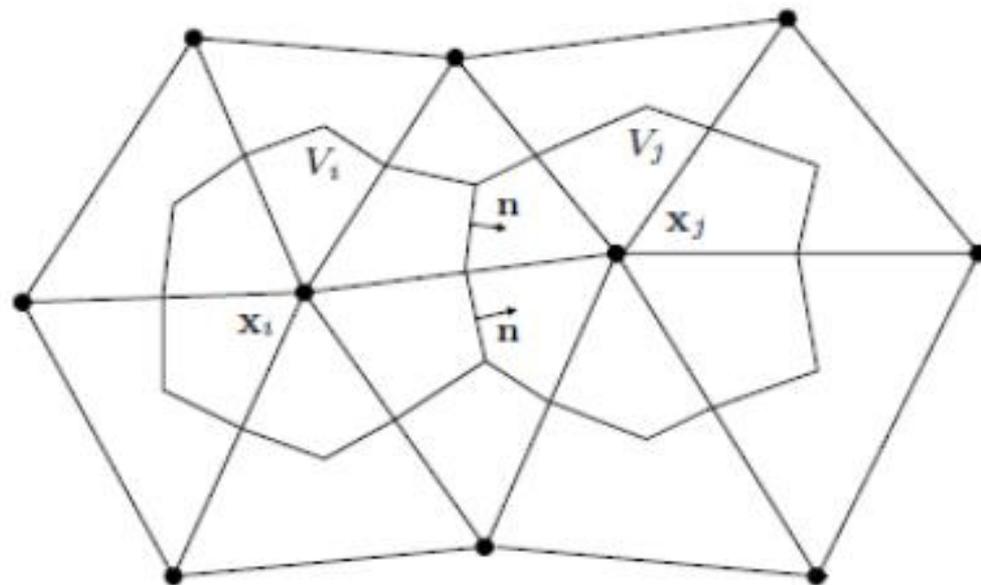


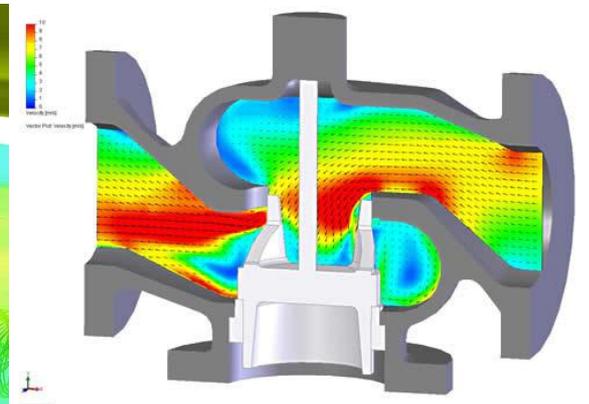
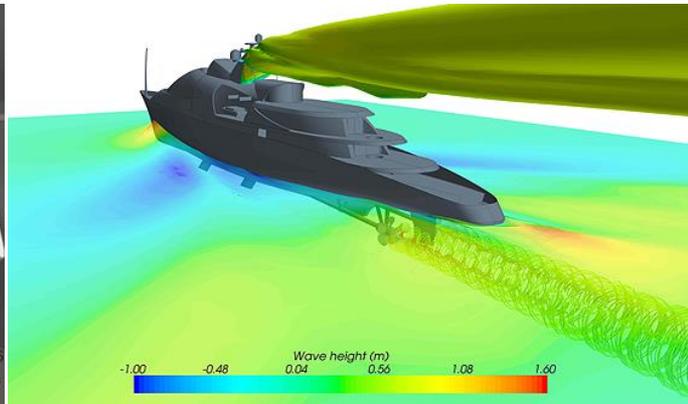
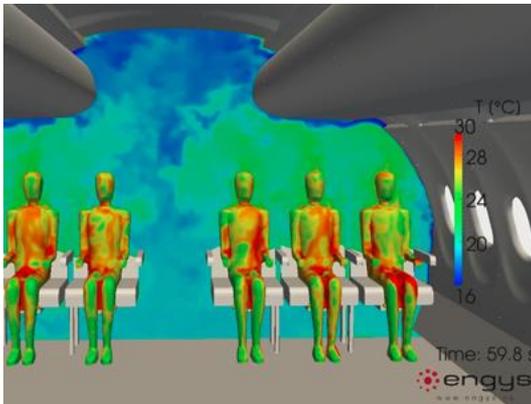
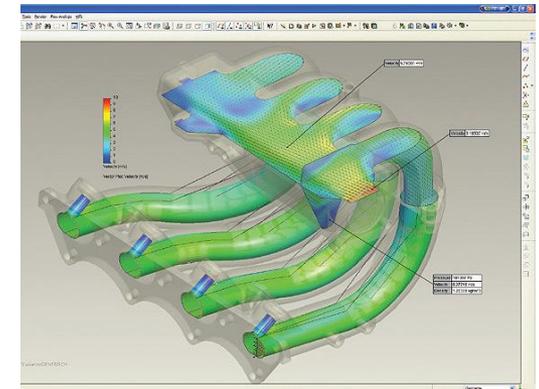
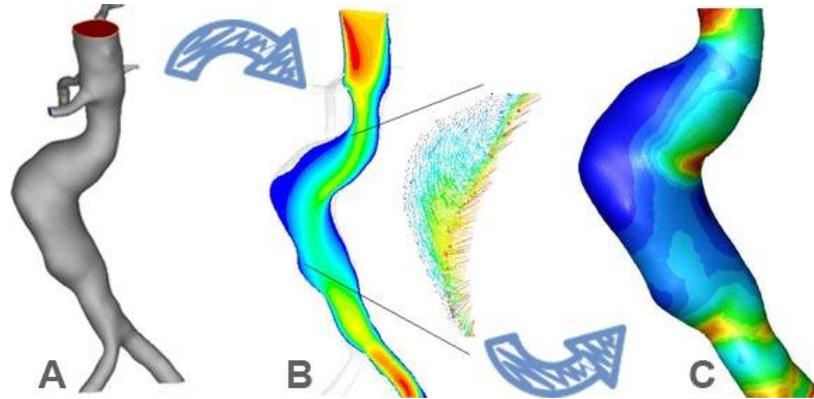
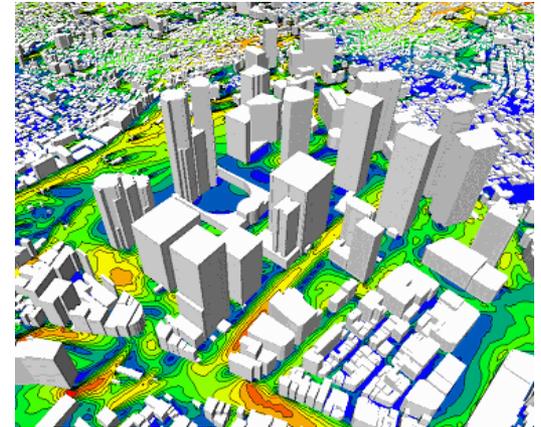
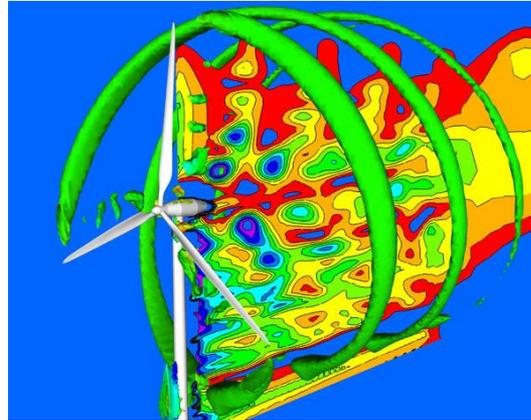
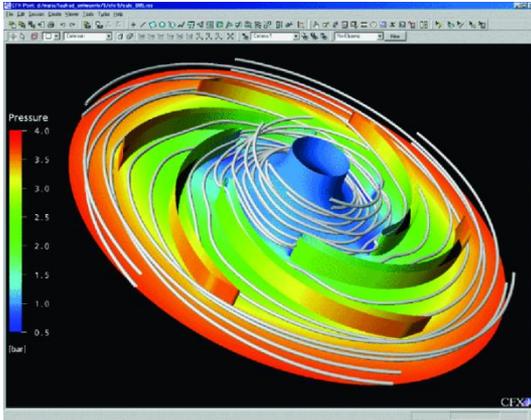
Fig. 1.6 Control volumes for a vertex-centered FVM in two dimensions.

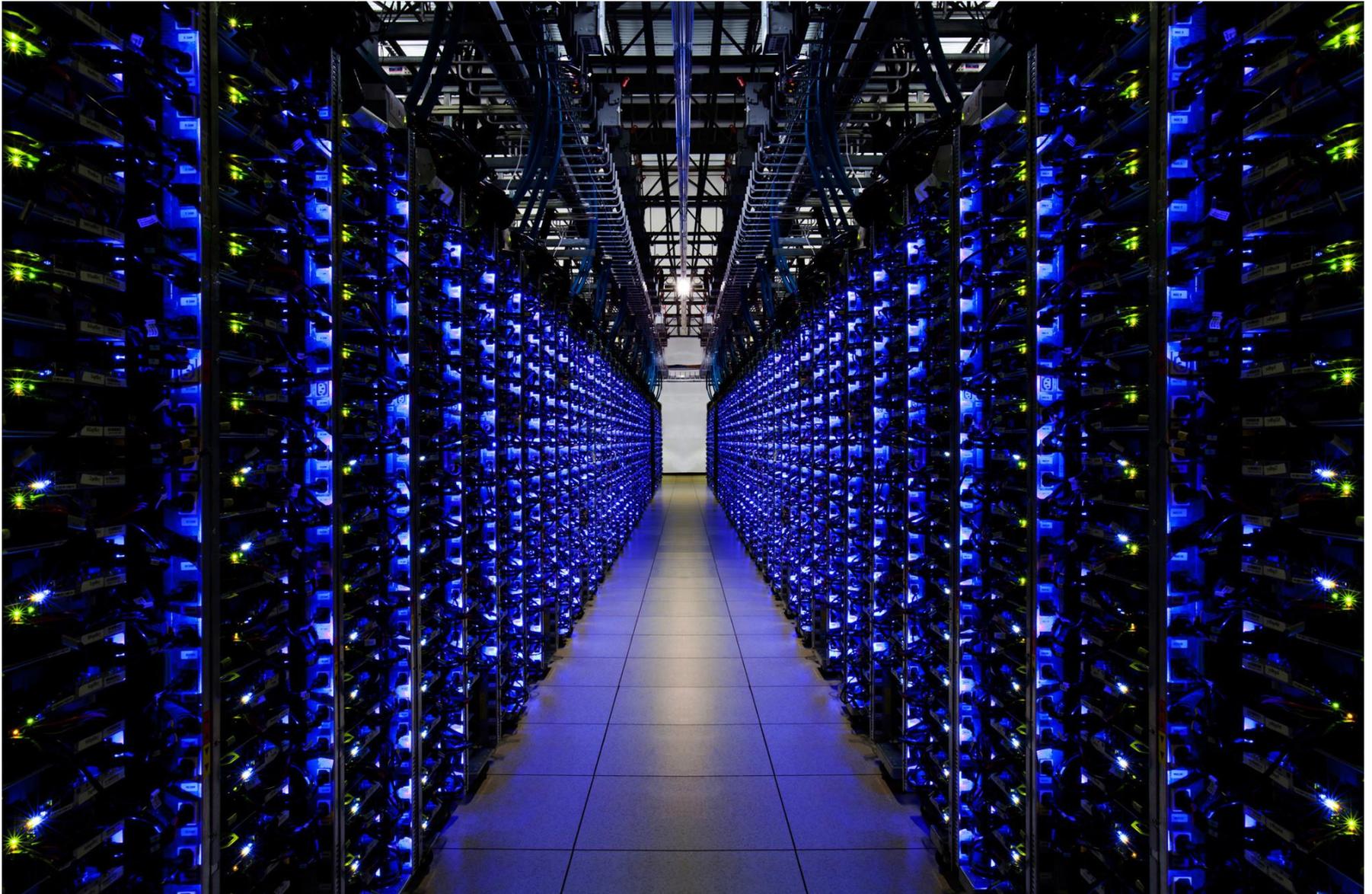


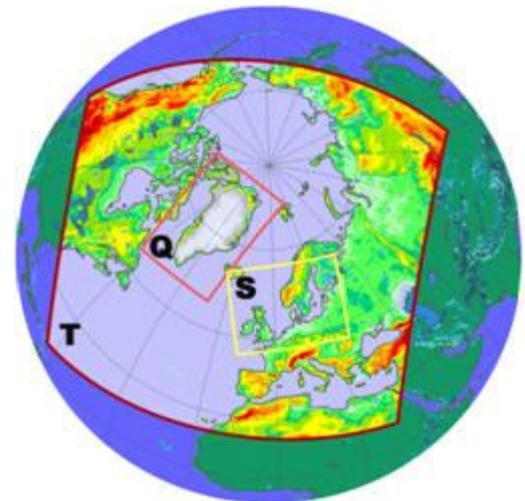
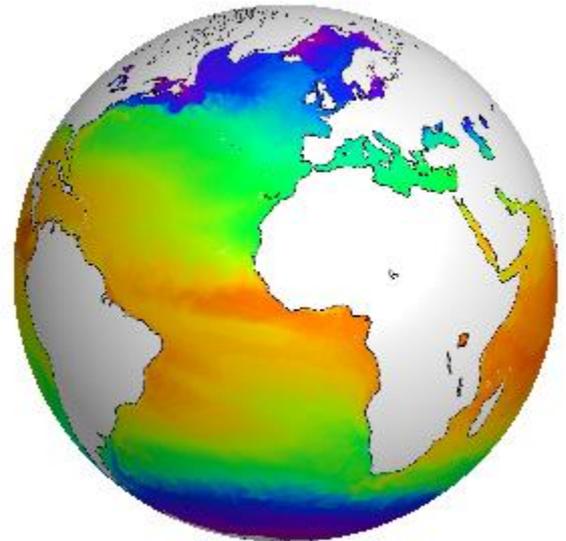
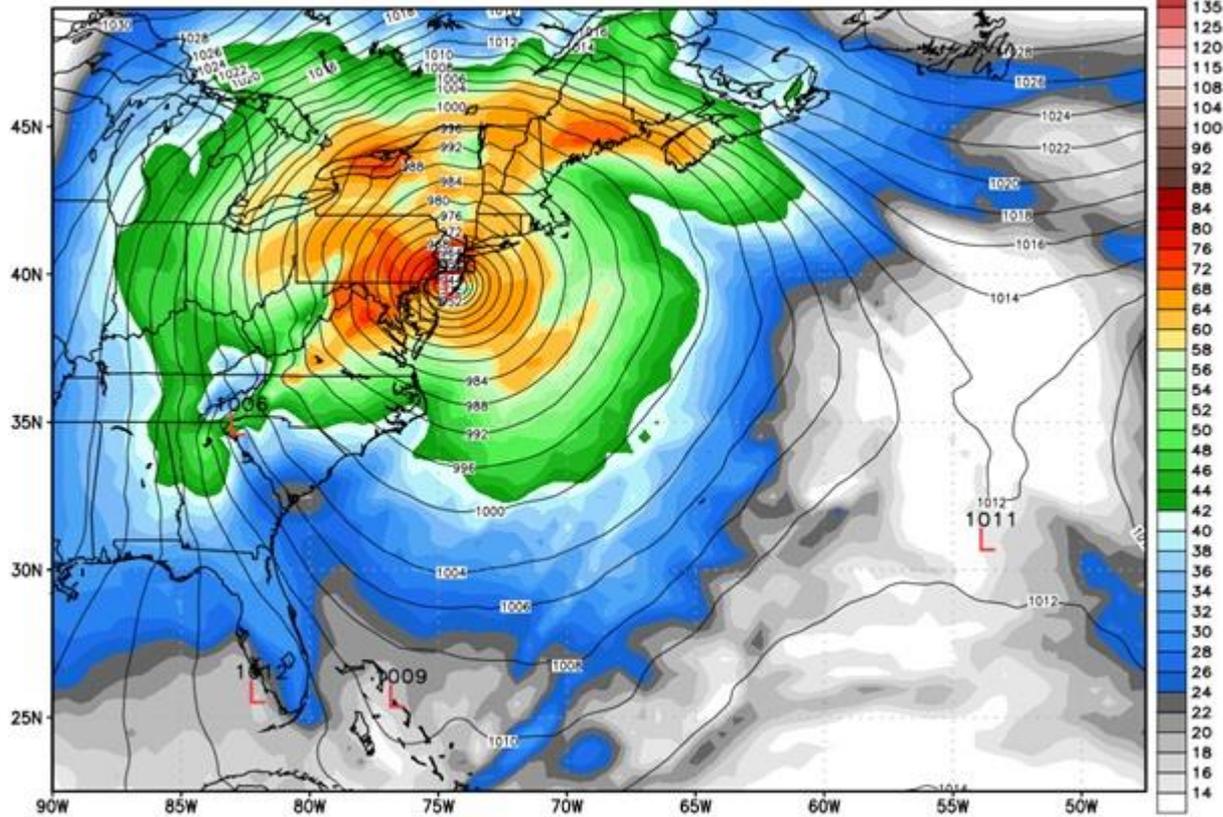
$$\frac{\partial}{\partial t} \int_{V_i} u(\mathbf{x}, t) \, d\mathbf{x} + \int_{S_i} (\mathbf{v}u - \mathcal{D}\nabla u) \cdot \mathbf{n} \, ds = \int_{V_i} s(\mathbf{x}, t) \, d\mathbf{x},$$

$$|V_i| \frac{du_i}{dt} + \sum_j \int_{S_{ij}} (\mathbf{v}u - \mathcal{D}\nabla u) \cdot \mathbf{n} \, ds = |V_i| s_i.$$

$$|V_i| \frac{du_i}{dt} + \sum_j (c_{ij} + d_{ij}) u_j = |V_i| s_i.$$







$$\frac{\partial u}{\partial t} + \dot{\sigma} \frac{\partial u}{\partial \sigma} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} - f v - \frac{uv}{r} \tan \phi + g \frac{\partial z}{\partial x} + c_p \theta \frac{\partial \pi}{\partial x} + F_x = 0$$

$$\frac{\partial v}{\partial t} + \dot{\sigma} \frac{\partial v}{\partial \sigma} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + f u + \frac{v^2}{r} \tan \phi + g \frac{\partial z}{\partial y} + c_p \theta \frac{\partial \pi}{\partial y} + F_y = 0$$

$$\frac{\partial(gz)}{\partial \sigma} + c_p \theta \frac{\partial \pi}{\partial \sigma} = 0,$$

$$\frac{\partial \theta}{\partial t} + \dot{\sigma} \frac{\partial \theta}{\partial \sigma} + u \frac{\partial \theta}{\partial x} + v \frac{\partial \theta}{\partial y} + H = 0,$$

$$\frac{\partial p_e}{\partial t} + \frac{\partial}{\partial \sigma} (\dot{\sigma} p_e) + \frac{\partial}{\partial x} (u p_e) + \frac{\partial}{\partial y} (v p_e) - \frac{v p_e}{r} \tan \phi = 0, \quad \pi = \left(\frac{p}{P}\right)^k.$$

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2º Semestre - 2020

Roteiro do curso

- Introdução
- Séries de Fourier
- **Método de Diferenças Finitas**
- Equação do calor transiente (parabólica)
- Equação de Poisson (elíptica)
- **Equação da onda (hiperbólica)**