

Meshfree models for simulation of reactive transport in groundwater systems

Aatish Anshuman & T.I. Eldho

Indian Institute of Technology Bombay , Mumbai, India



Research motivation



Results



Methodology



Concluding remarks



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Research motivation



Reactive contaminants enter the groundwater through different sources.

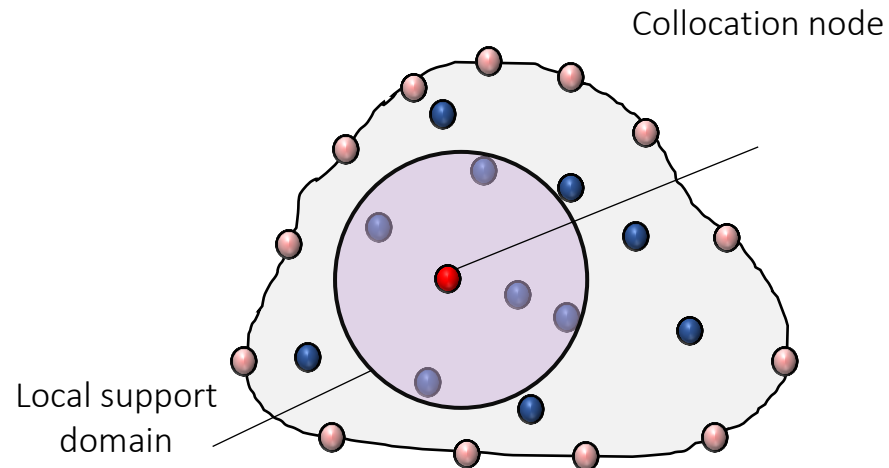


Existing simulation models (FDM & FEM) based on mesh/grid face following issues

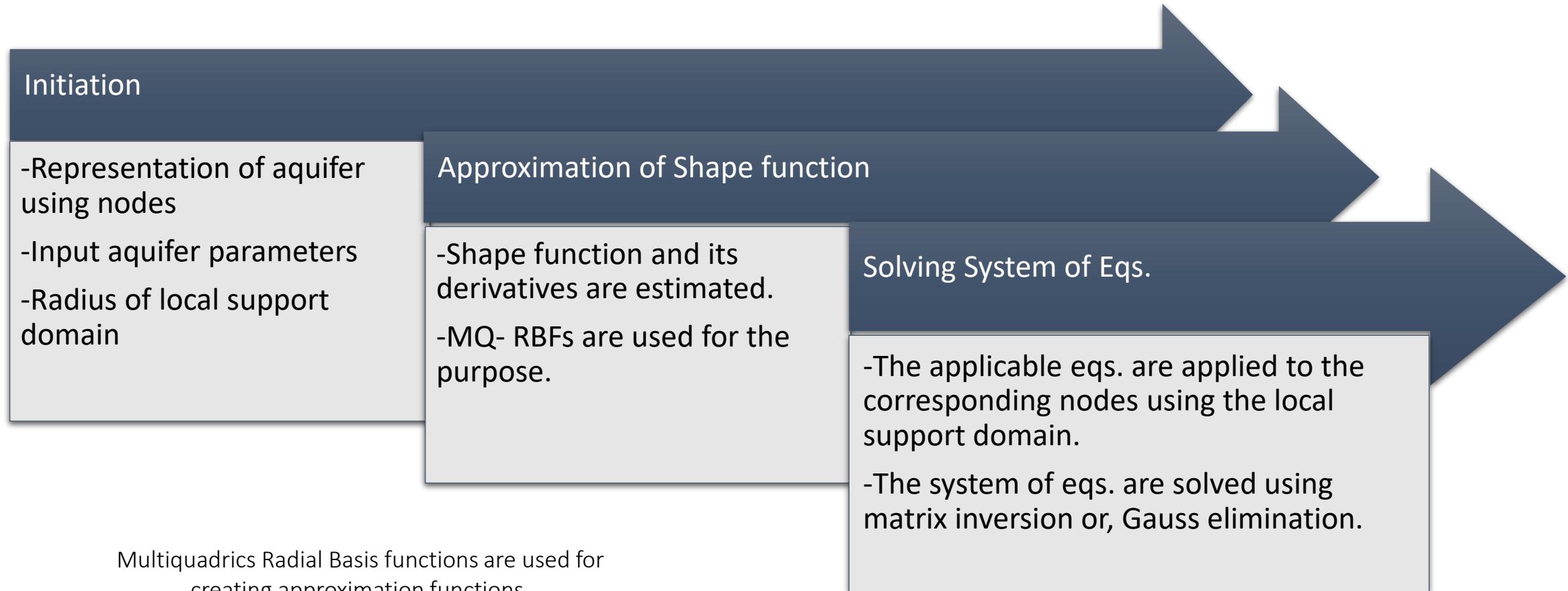
- ✓ Instability in high advection problems
- ✓ Unsuitable for highly irregular boundary
- ✓ Not adaptable for dynamic node creation
- ✓ Use of operator splitting for transport components



Meshfree models handle these issues by eliminating the mesh and using a **support domain** for node-to-node transfer of state variables.



Methodology



Multiquadrics Radial Basis functions are used for creating approximation functions.

$$R(x) = (r + (\alpha d_c)^2)^q$$

r-radial distance

q, α -shape parameters

d_c -average nodal distance



Results



First order decay network



Non linear adsorption



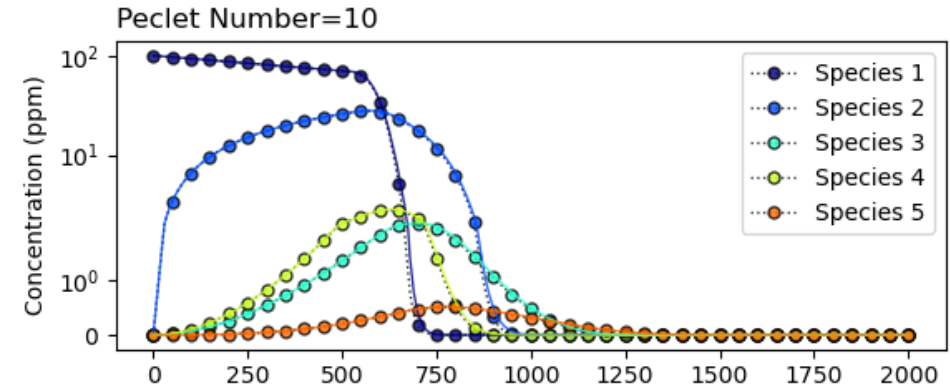
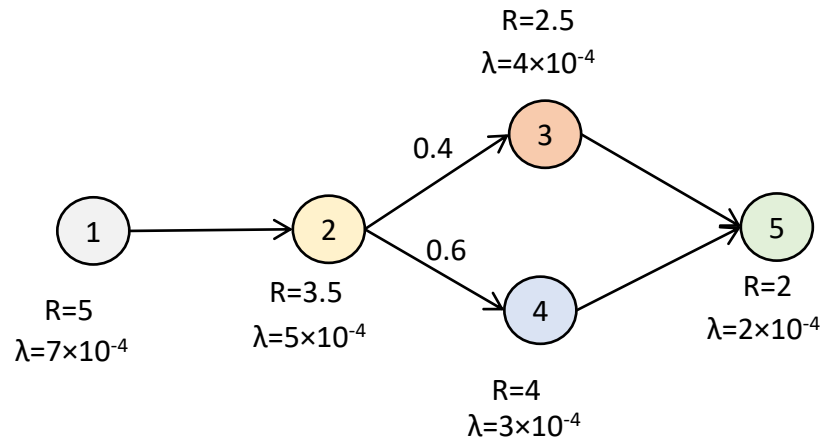
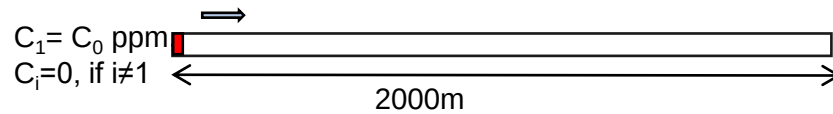
First order decay network

Governing equation

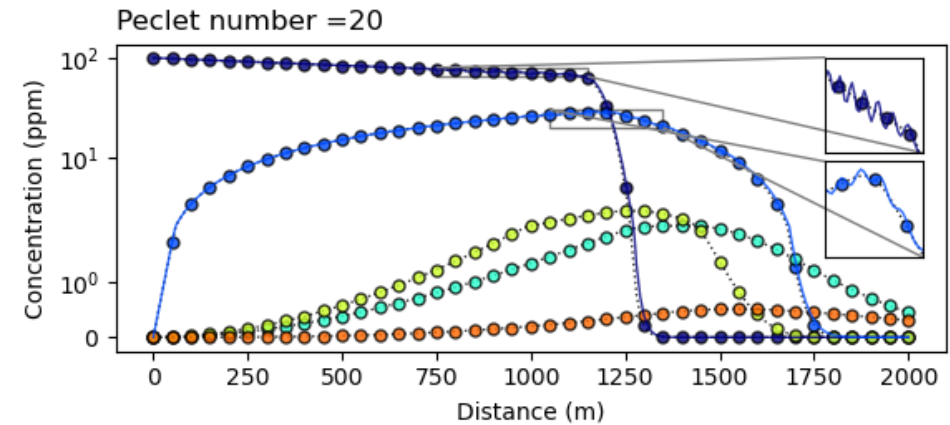
$$R \frac{\partial C_i}{\partial t} = \frac{\partial}{\partial x} \left[D_{xx} \frac{\partial C_i}{\partial x} \right] - \frac{\partial (V_x C_i)}{\partial x} - R \lambda_i C_i + \frac{q_w C_i}{n_e B} + \lambda_{i-1} C_{i-1}$$

C= contaminant concentration
R= Retardation factor
D=Dispersion coefficient
V=seepage velocity

λ =1st order decay rate
 n_e =porosity
B=depth
 q_w =injection rate



$V=1\text{m/d}$
 $D=1\text{m}^2/\text{d}$



$V=2\text{m/d}$
 $D=1\text{m}^2/\text{d}$

Comparison between RPCM and FEM

- ✓ FEM solutions(dotted lines) show instability for high advection
- ✓ RPCM (solid lines) solutions are stable



Nonlinear adsorption

Governing equation

$$\left\{ 1 + \frac{\rho_b}{n_e} \cdot \frac{K_L \cdot S_{max}}{(1 + K_L \cdot C)^2} \right\} \frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left[D_{xx} \frac{\partial C}{\partial x} \right] - \frac{\partial(V_x C)}{\partial x} + \frac{q_w C_i}{n_e B}$$

C= contaminant concentration

S=adsorbed concentration

D=Dispersion coefficient

V=seepage velocity

n_e =porosity

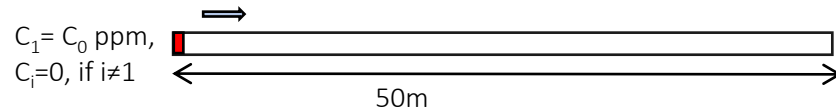
B=depth

q_w =injection rate

K_L =Langmuir const.

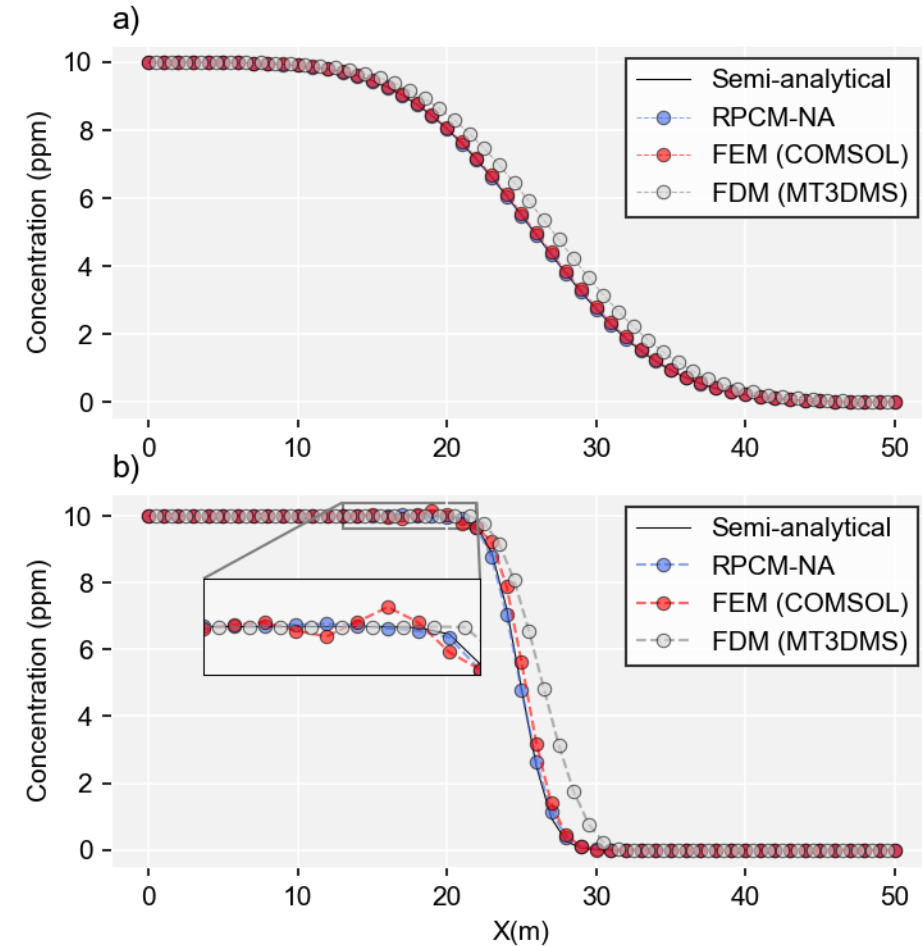
S_{max} =Max. adsorption capacity

ρ_b =bulk density of soil



- K_L and S_{max} values are fixed as 0.0001 L/mg and 1 mg/g respectively
- The bulk density and porosity of the soil are 1400 kg/m³ and 0.3 respectively.
- The velocity of flow is 0.2 m/d
- The dispersion coefficient is varied to vary the Peclet number ($Pe = v \cdot \Delta x / D$)
- Model performance is compared against semi analytical solution (Serrano, 2001)

- ✓ RPCM model performs well for both cases.
- ✓ For high Pe, FEM model shows oscillations and FDM shows numerical dispersion.
- ✓ FDM model shows numerical dispersion for both cases which increase with Pe value.



Comparison of model simulations after 1 year for
Pe=1 (case a), Pe=20 case b)



Concluding remarks

- ✓ RPCM based meshfree models are effective for simulating reactive transport in groundwater.
- ✓ These models eliminate the use of mesh and thus deal with related instability such as artificial oscillations and numerical dispersion.
- ✓ These models are flexible for dynamic node generation and deal with irregular boundaries effectively.
- ✓ These models have also been applied field scale aquifers.



Contact



Aatish Anshuman



aatishanshuman@gmail.com



References

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2. Anshuman, A., & Eldho, T. I. (2019). Modeling of transport of first-order reaction networks in porous media using meshfree radial point collocation method. *Computational Geosciences*, 23(6), 1369-1385.
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